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IN THE UNITED STATES PATENT & TRADEMARK OFFICE

IN RE APPLICATION OF:
WILLIS ET AL.

:

: GROUP ART UNIT: **3746**
(ANTICIPATED)

SERIAL NO.: NEW APPLICATION

:

FILED: HEREWITH

: EXAMINER: **LOUIS J. CASAREGOLA**
(REQUESTED)

FOR: INTEGRATED TURBINE POWER GENERATION
SYSTEM HAVING LOW PRESSURE SUPPLEMENTAL
CATALYTIC REACTOR

ASSISTANT COMMISSIONER FOR PATENTS
WASHINGTON, D.C. 20231

SIR:

REQUEST FOR SPECIFIC EXAMINER
REGARDING **COPIED CLAIMS**

*I request that this application be assigned to Primary Examiner **LOUIS J.***

CASAREGOLA, in group art unit 3764 because (1) he examined **the exact same claims** as claims 1-2 presented herein when he examined and allowed United States patent No. 6,205,768 and (2) because this application raises interference issues requiring the attention of a primary examiner knowledgeable in this technology.

Claims 1-3 in this application are identical copies of (1) claims 1 and 2 in United States patent No. 6,205,768, issued March 27, 2001, naming Robert W.Dibble and Rajiv K.Mongia as

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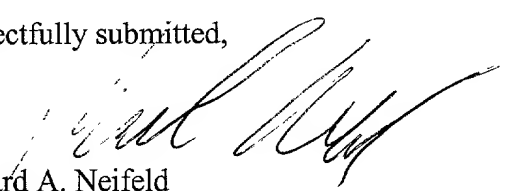
inventors, and assigned at issue to Solo Energy Corporation, and (2) claim 1 in United States patent No. 6,109,693 issued August 22, 2000, naming Rajiv K. Mongia, George L. Touchon, Robert W. Dibble, and Martin L. Lagod as inventors, and assigned at issue to Solo Energy Corporation. This application supports the limitations defined in claims 1-3; see for example Figure 3 showing separate air and fuel lines 18, 46, the compressor 4, the recuperator 12, the primary catalytic converter 14, the turbine 10, and the low pressure catalytic converter 16.

In addition, claims 4-9 are modeled after the three claims identified above in the '768 and '693 patents.

I intend to file a 37 CFR 1.607 interference request with those two patents as soon as practicable after filing this application.

Since this application raises interference issues, *it should be placed on the examiner's special cases docket.*

Respectfully submitted,


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Appendix A

POWER CONTROLLER

REFERENCE TO RELATED APPLICATION

This application claims the benefit of U.S. Provisional Application No. 60/080,457, filed on April 2, 1998.

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BACKGROUND OF THE INVENTION

1. Field of the Invention

This invention relates generally to power generation and processing systems and in particular to distributed generation power systems.

2. Description of the Prior Art

Conventional power generation and distribution systems are configured to maximize the specific hardware used. In the case of a turbine power motor, for example, the output or bus voltage in a conventional power distribution system varies with the speed of the turbine. In such systems, the turbine speed must be regulated to control the output or bus voltage. Consequently, the engine cannot be run too low in speed else the bus voltage would not be high enough to generate some of the voltages that are needed. As a result, the turbine would have to be run at higher speeds and lower temperatures, making it less efficient.

What is needed therefore is a power generation and distribution system where the bus voltage is regulated by a bi-directional controller independent of turbine speed.

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SUMMARY OF THE INVENTION

The present invention provides in a first aspect, a power controller which provides a distributed generation power networking system in which bi-directional power converters are used with a common DC bus for permitting compatibility

between various energy components. Each power converter operates essentially as a customized bi-directional switching converter configured, under the control of the power controller, to provide an interface for a specific energy component to the DC bus. The power controller controls the way in which each energy component, at any moment, will sink or source power, and the manner in which the DC bus is regulated. In this way, various energy components can be used to supply, store and/or use power in an efficient manner. The various energy components include energy sources, loads, storage devices and combinations thereof.

In another aspect, the present invention provides a turbine system including a turbine engine, a load, a power controller, an energy reservoir for providing transient power to the DC bus and an energy reservoir controller, in communication with the power controller for providing control to the energy reservoir. The power controller includes an engine power conversion in communication with the turbine engine, an utility power conversion in communication with the load and a DC bus.

These and other features and advantages of this invention will become further apparent from the detailed description and accompanying figures that follow. In the figures and description, numerals indicate the various features of the invention, like numerals referring to like features throughout both the drawing figures and the written description.

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 is a block diagram of a power controller according to the present invention.

FIG. 2 is a detailed block diagram of a power converter in the power controller illustrated in FIG. 1.

FIG. 3 is a simplified block diagram of a turbine system including the power architecture of the power controller illustrated in FIG. 1.

FIG. 4 is a block diagram of the power architecture of a typical implementation of the power controller illustrated in FIG. 1.

FIG. 5 is a schematic diagram of the internal power architecture of the power controller illustrated in FIG. 1.

FIG. 6 is a functional block diagram of an interface between load/utility grid and turbine generator using the power controller according to the present invention.

FIG. 7 is a functional block diagram of an interface between load/utility grid and turbine generator using the power controller for a stand-alone application according to the present invention.

FIG. 8 is a schematic diagram of an interface between a load/utility grid and turbine generator using the power controller according to the present invention.

FIG. 9 is a block diagram of the software architecture for the power controller including external interfaces.

FIG. 10 is a block diagram of an EGT control mode loop for regulating the temperature of the turbine.

FIG. 11 is a block diagram of a speed control mode loop for regulating the rotating speed of the turbine.

FIG. 12 is a block diagram of a power control mode loop for regulating the power producing potential of the turbine.

FIG. 13 is a state diagram showing various operating states of the power controller.

FIG. 14 is a block diagram of the power controller interfacing with a turbine and fuel device.

FIG. 15 is a block diagram of the power controller in multi-pack configuration.

FIG. 16 is a block diagram of a utility grid analysis system for the power controller according to the present invention.

FIG. 17 is a graph of voltage against time for the utility grid analysis system illustrated in FIG. 16.

FIG. 18 is a diagram of the power controller shown in FIG. 16, including brake resistor.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENT(S)

Referring to FIG.1, power controller 10 provides a distributed generation power networking system in which bi-directional (i.e. reconfigurable) power converters are

used with a common DC bus for permitting compatibility between one or more energy components. Each power converter operates essentially as a customized bi-directional switching converter configured, under the control of power controller 10, to provide an interface for a specific energy component to DC bus 24. Power controller 10 controls the way in which each energy component, at any moment, will sink or source power, and the manner in which DC bus 24 is regulated. In this way, various energy components can be used to supply, store and/or use power in an efficient manner.

One skilled in the art will recognize that the particular configurations shown herein are for illustrative purposes only. In particular, the present invention is not limited to the use of three bi-directional converters as shown in FIG. 1. Rather, the number of power converters is dependent on various factors, including but not limited to, the number of energy components and the particular power distribution configuration desired. For example, as illustrated in FIGS. 5 and 6, power controller 10 can provide a distributed generation power system with as few as two power converters.

The energy components, as shown in FIG. 1, include energy source 12, utility/load 18 and storage device 20. The present invention is not limited to the distribution of power between energy source 12, energy storage device 20 and utility/load 18, but rather may be adapted to provide power distribution in an efficient manner for any combination of energy components.

Energy source 12 may be a gas turbine, photovoltaics, wind turbine or any other conventional or newly developed source. Energy storage device 20 may be a flywheel, battery, ultracap or any other conventional or newly energy storage device. Load 18 may be an utility grid, dc load, drive motor or any other conventional or newly developed utility/load 18.

Referring now to FIG. 2, a detailed block diagram of power converter 14 in power controller 10, shown in FIG. 1, is illustrated. Energy source 12 is connected to DC bus 24 via power converter 14. Energy source 12 may be, for example, a gas turbine driving an AC generator to produce AC which is applied to power converter 14. DC bus 24 connects power converter 14 to utility/load 18 and additional energy components 36. Power converter 14 includes input filter 26, power switching system

28, output filter 34, signal processor 30 and main CPU 32. In operation, energy source 12 applies AC to input filter 26 in power converter 14. The filtered AC is then applied to power switching system 28 which may conveniently be a series of insulated gate bipolar transistor (IGBT) switches operating under the control of signal processor (SP) 30 which is controlled by main CPU 32. One skilled in the art will recognize that other conventional or newly developed switches may be utilized as well. The output of the power switching system 28 is applied to output filter 34 which then applies the filtered DC to DC bus 24.

In accordance with the present invention, each power converter 14, 16 and 22 operates essentially as a customized, bi-directional switching converter under the control of main CPU 32, which uses SP 30 to perform its operations. Main CPU 32 provides both local control and sufficient intelligence to form a distributed processing system. Each power converter 14, 16 and 22 is tailored to provide an interface for a specific energy component to DC bus 24. Main CPU 32 controls the way in which each energy component 12, 18 and 20 sinks or sources power, and DC bus 24 is regulated at any time. In particular, main CPU 32 reconfigures the power converters 14, 16 and 22 into different configurations for different modes of operation. In this way, various energy components 12, 18 and 20 can be used to supply, store and/or use power in an efficient manner. In the case of a turbine power generator, for example, a conventional system regulates turbine speed to control the output or bus voltage. In the power controller, the bi-directional controller independently of turbine speed regulates the bus voltage.

Operating Modes

FIG. 1 shows the system topography in which DC bus 24, regulated at 800 v DC for example, is at the center of a star pattern network. In general, energy source 12 provides power to DC bus 24 via power converter 14 during normal power generation mode. Similarly, during the power generation mode, power converter 16 converts the power on DC bus 24 to the form required by utility/load 18, which may be any type of load including a utility web. During other modes of operation, such as utility start up, power converters 14 and 16 are controlled by the main processor to operate in different manners.

For example, energy is needed to start the turbine. This energy may come from load/utility grid 18 (utility start) or from energy storage 20 (battery start), such as a battery, flywheel or ultra-cap. During a utility start up, power converter 16 is required to apply power from load 18 to DC bus 24 for conversion by power converter 14 into the power required by energy source 12 to startup. During utility start, energy source or turbine 12 is controlled in a local feedback loop to maintain the turbine revolutions per minute (RPM). Energy storage or battery 20 is disconnected from DC bus 24 while load/utility grid 10 regulates V_{DC} on DC bus 24.

Similarly, in the battery start mode, the power applied to DC bus 24 from which energy source 12 is started may be provided by energy storage 20 which may be a flywheel, battery or similar device. Energy storage 20 has its own power conversion circuit in power converter 22, which limits the surge current into DC bus 24 capacitors, and allows enough power to flow to DC Bus 24 to start energy source 12. In particular, power converter 16 isolates DC bus 24 so that power converter 14 can provide the required starting power from DC bus 24 to energy source 12.

Electronics Architecture

Referring to FIG. 3, a simplified block diagram of a turbine system 50 using the power controller electronics architecture of the present invention is illustrated. The turbine system 50 includes a fuel metering system 42, turbine engine 58, power controller 52, energy reservoir conversion 62, energy/reservoir 64 and load/utility grid 60. The fuel metering system 42 is matched to the available fuel and pressure. The power controller 52 converts the electricity from turbine engine 58 into regulated DC then converts it to utility grade AC electricity. By separating the engine control from the converter that creates the utility grade power, greater control of both processes is realized. All of the interconnections are comprised of a communications bus and a power connection.

The power controller 52 includes an engine power conversion 54 and utility power conversion 56 which provides for the two power conversions that take place between the turbine 58 and the load/utility grid 60. One skilled in the art will recognize that the power controller 52 can provide a distributed generation power system with as few as two power converters 54 and 56. The bi-directional (i.e. reconfigurable) power

converters 54 and 56 are used with a common regulated DC bus 66 for permitting compatibility between the turbine 58 and load/utility grid 60. Each power converter 54 and 56 operates essentially as a customized bi-directional switching converter configured, under the control of the power controller 10, to provide an interface for a specific energy component 58 or 60 to the DC bus 66. The power controller 10 controls the way in which each energy component, at any moment, will sink or source power, and the manner in which the DC bus 66 is regulated. Both of these power conversions 54 and 56 are capable of operating in a forward or reverse direction. This allows starting the turbine 58 from either the energy reservoir 64 or the load/utility grid 60. The regulated DC bus 66 allows a standardized interface to energy reservoirs such as batteries, flywheels, and ultra-caps. The architecture of the present invention permits the use of virtually any technology that can convert its energy to/from electricity. Since the energy may flow in either direction to or from the energy reservoir 64, transients may be handled by supplying energy or absorbing energy. Not all systems will need the energy reservoir 64. The energy reservoir 64 and its energy reservoir conversion 62 are not contained inside the power controller 52.

Referring to FIG. 4, the power architecture 68 of a typical implementation of the power controller 70 is shown. The power controller 70 includes a generator converter 72 and output converter 74 which provides for the two power conversions that take place between the turbine 76 and the load/utility grid 78. In particular, the generator converter 72 provides for AC to DC power conversion and the output converter 74 provides for DC to AC power conversion. Both of these power converters 72 and 74 are capable of operating in a forward or reverse direction. This allows starting the turbine 76 from either the energy storage device 86 or the load/utility grid 78. Since the energy may flow in either direction to or from the energy storage device 86, transients may be handled by supplying energy or absorbing energy. The energy storage device 86 and its DC converter 84 are not contained inside the power controller 70. The DC converter 84 provides for DC to DC power conversion.

Referring to FIG. 5, a schematic 90 of a typical internal power architecture, such as that shown in FIG. 4, is shown. The turbine has an integral PMG that can be used as either a generator (for starting) or a generator (normal mode of operation).

Because all of the controls can be performed in the digital domain and all switching (except for one output contactor) is done with solid state switches, it is easy to shift the direction of the power flow as needed. This permits very tight control of the turbine during starting and stopping. In a typical configuration, the power output is a 480

- 5 VAC, 3-phase output. One skilled in the art will recognize that the present invention may be adapted to provide for other power output requirements such as a 3-phase, 400 VAC, and single-phase, 480 VAC.

Power controller 92 includes generator converter 94 and output converter 96. Generator converter 94 includes IGBT switches 94, such as a seven-pack IGBT module
10 94, driven by control logic 98, providing a variable voltage, variable frequency 3-phase drive to the PMG 100. Inductors 102 are utilized to minimize any current surges associated with the high frequency switching components which may affect the PMG 100 to increase operating efficiency.

IGBT module 94 is part of the electronics that controls the engine of the
15 turbine. IGBT module 94 incorporates gate driver and fault sensing circuitry as well as a seventh IGBT used to dump power into a resistor. The gate drive inputs and fault outputs require external isolation. Four external, isolated power supplies are required to power the internal gate drivers. IGBT module 94 is typically used in a turbine system that generates 480 VAC at its output terminals delivering up to 30 kWatts to a
20 freestanding or utility-connected load. During startup and cool down (and occasionally during normal operation), the direction of power flow through the seven-pack reverses. When the turbine is being started, power is supplied to the DC bus 112 from either a battery (not shown) or from the utility grid 108. The DC is converted to a variable frequency AC voltage to generator the turbine.

25 For utility grid connect operation, control logic 110 sequentially drives the solid state IGBT switches, typically configured in a six-pack IGBT module 96, associated with load converter 96 to boost the utility voltage to provide start power to the generator converter 94. The IGBT switches in load converter 96 are preferably operated at a high (15 kHz) frequency, and modulated in a pulse width modulation
30 manner to provide four quadrant converter operation. Inductors 104 and AC filter

capacitors 106 are utilized to minimize any current surges associated with the high frequency switching components which may affect load 108.

Six-pack IGBT module 96 is part of the electronics that controls the converter of the turbine. IGBT module 96 incorporates gate driver and fault sensing circuitry.

- 5 The gate drive inputs and fault outputs require external isolation. Four external, isolated power supplies are required to power the internal gate drivers. IGBT module 96 is typically used in a turbine system that generates 480 VAC at its output terminals delivering up to approximately 30 kWatts to a free-standing or utility-connected load. After the turbine is running, six-pack IGBT module 96 is used to convert the regulated
- 10 DC bus voltage to the approximately 50 or 60 hertz utility grade power. When there is no battery (or other energy reservoir), the energy to run the engine during startup and cool down must come from utility grid 108. Under this condition, the direction of power flow through the six-pack IGBT module 96 reverses. DC bus 112 receives its energy from utility grid 108, using six-pack IGBT module 96 as a boost converter (the
- 15 power diodes act as a rectifier). The DC is converted to a variable frequency AC voltage to generator the turbine. To accelerate the engine as rapidly as possible at first, current flows at the maximum rate through seven-pack IGBT module 94 and also six-pack IGBT module 96.

- 20 Dual IGBT module 114, driven by control logic 116, is used to provide an optional neutral to supply 3 phase, 4 wire loads.

Startup

- 25 Energy is needed to start the turbine. Referring to FIGS. 3 and 4, this energy may come from utility grid 60 or from energy reservoir 64, such as a battery, flywheel or ultra-cap. When utility grid 60 supplies the energy, utility grid 60 is connected to power controller 52 through two circuits. First is an output contactor that handles the full power (30 kWatts). Second is a "soft-start" or "pre-charge" circuit that supplies limited power (it is current limited to prevent very large surge currents) from utility grid 66 to DC bus 62 through a simple rectifier. The amount of power supplied through the soft-start circuit is enough to start the housekeeping power supply, power
- 30 the control board, and run the power supplies for the IGBTs, and close the output contactor. When the contactor closes, the IGBTs are configured to create DC from the

AC waveform. Enough power is created to run the fuel metering circuit 42, start the engine, and close the various solenoids (including the dump valve on the engine).

When energy reservoir 64 supplies the energy, energy reservoir 64 has its own power conversion circuit 62 that limits the surge circuit into DC bus capacitors.

- 5 Energy reservoir 64 allows enough power to flow to DC bus 62 to run fuel-metering circuit 42, start the engine, and close the various solenoids (including the dump valve on the engine). After the engine becomes self-sustaining, the energy reservoir starts to replace the energy used to start the engine, by drawing power from DC bus 62. In addition to the sequences described above, power controller senses the presence of
- 10 other controllers during the initial power up phase. If another controller is detected, the controller must be part of a multi-pack, and proceeds to automatically configure itself for operation as part of a multi-pack.

System Level Operation

- Referring to FIG. 6, a functional block diagram 130 of an interface between
- 15 utility grid 132 and turbine generator 148 using power controller 136 of the present invention is shown. In this example, power controller 136 includes two bi-directional converters 138 and 140. Permanent magnet generator converter 140 starts turbine 148 (using the generator as a generator) from utility or battery power. Load converter 138 then produces AC power using an output from generator converter 140 to draw power
- 20 from high-speed turbine generator 148. Power controller 136 also regulates fuel to turbine 148 and provides communications between units (in paralleled systems) and to external entities.

- During a utility startup sequence, utility 132 supplies starting power to turbine 148 by "actively" rectifying the line via load converter 138, and then converting the
- 25 DC to variable voltage, variable frequency 3-phase power in generator converter 136. As is illustrated in FIG. 7, for stand-alone applications 150, the start sequence is the same as the utility start sequence shown in FIG. 6 with the exception that the start power comes from battery 170 under the control of an external battery controller. Load 152 is then fed from the output terminals of load converter 158.

- 30 Referring to FIG. 8, a schematic illustration 180 of an interface between utility grid 132 and turbine generator 148 using the power controller is illustrated. Control

logic 184 also provides power to fuel cutoff solenoids 198, fuel control valve 200 and igniter 202. An external battery controller (not shown), if used, connects directly to DC bus 190. In accordance with an alternative embodiment of the invention, a fuel system (not shown) involving a compressor (not shown) operated from a separate variable speed drive can also derive its power directly from DC bus 190.

In operation, control and start power comes from either the external battery controller (for battery start applications) or from the utility, which is connected to a rectifier using inrush limiting techniques to slowly charge internal bus capacitor 190. For utility grid connect operation, control logic 184 sequentially drives solid state IGBT switches 214 associated with load converter 192 to boost the utility voltage to provide start power to generator converter 186. Switches 214 are preferably operated at a high (15 kHz) frequency, and modulated in a pulse width modulation manner to provide four quadrant converter operation. In accordance with the present invention, load converter 192 either sources power from DC bus 190 to utility grid 222 or from utility grid 222 to DC bus 190. A current regulator (not shown) may achieve this control. Optionally, two of the switches 214 serve to create an artificial neutral for stand-alone applications (for stand-alone applications, start power from an external DC supply (not shown) associated with external DC converter 220 is applied directly to DC bus 190).

Solid state (IGBT) switches 214 associated with generator converter 186 are also driven from control logic 184, providing a variable voltage, variable frequency 3-phase drive to generator 218 to start turbine 208. Control logic 184 receives feedback via current sensors I_{sens} as turbine 206 is ramped up in speed to complete the start sequence. When turbine 206 achieves a self sustaining speed of, for example, approx. 40,000 RPM, generator converter 186 changes its mode of operation to boost the generator output voltage and provide a regulated DC bus voltage.

PMG filter 188 associated with generator converter 186 includes three inductors to remove the high frequency switching component from permanent magnet generator 208 to increase operating efficiency. Output AC filter 194 associated with load converter 192 includes three or optionally four inductors (not shown) and AC

filter capacitors (not shown) to remove the high frequency switching component. Output contactor 210 disengages load converter 192 in the event of a unit fault.

During a start sequence, control logic 184 opens fuel cutoff solenoid 198 and maintains it open until the system is commanded off. Fuel control 200 may be a variable flow valve providing a dynamic regulating range, allowing minimum fuel during start and maximum fuel at full load. A variety of fuel controllers, including but not limited to, liquid and gas fuel controllers, may be utilized. One skilled in the art will recognize that the fuel control can be by various configurations, including but not limited to a single or dual stage gas compressor accepting fuel pressures as low as approximately ¼ psig. Igniter 202, a spark type device similar to a spark plug for an internal combustion engine, is operated only during the start sequence.

For stand-alone operation, turbine 206 is started using external DC converter 220 which boosts voltage from a battery (not shown), and connects directly to the DC bus 190. Load converter 192 is then configured as a constant voltage, constant frequency (for example, approximately 50 or 60 Hz) source. One skilled in the art will recognize that the output is not limited to a constant voltage, constant frequency source, but rather may be a variable voltage, variable frequency source. For rapid increases in output demand, external DC converter 220 supplies energy temporarily to DC bus 190 and to the output. The energy is restored after a new operating point is achieved.

For utility grid connect operation, the utility grid power is used for starting as described above. When turbine 206 has reached a desired operating speed, converter 192 is operated at utility grid frequency, synchronized with utility grid 222, and essentially operates as a current source converter, requiring utility grid voltage for excitation. If utility grid 222 collapses, the loss of utility grid 222 is sensed, the unit output goes to zero (0) and disconnects. The unit can receive external control signals to control the desired output power, such as to offset the power drawn by a facility, but ensure that the load is not backfed from the system.

Power Controller Software

Referring to FIG. 9, power controller 230 includes main CPU 232, generator SP 234 and converter SP 236. Main CPU software program sequences events which occur

inside power controller 230 and arbitrates communications to externally connected devices. Main CPU 232 is preferably a MC68332 microprocessor, available from Motorola Semiconductor, Inc. of Phoenix, Arizona. Other suitable commercially available microprocessors may be used as well. The software performs the algorithms that control engine operation, determine power output and detect system faults.

Commanded operating modes are used to determine how power is switched through the major converts in the controller. The software is responsible for turbine engine control and issuing commands to other SP processors enabling them to perform the generator converter output converter power switching. The controls also interface with externally connected energy storage devices (not shown) that provide black start and transient capabilities.

Generator SP 234 and converter SP 236 are connected to power controller 230 via serial peripheral interface (SPI) bus 238 to perform generator and converter control functions. Generator SP 234 is responsible for any switching which occurs between DC bus 258 and the output to generator. Converter SP 236 is responsible for any switching which occurs between DC bus 258 and output to load. As illustrated in FIG. 5, generator SP 234 and converter SP 236 operate IGBT modules.

Local devices, such as a smart display 242, smart battery 244 and smart fuel control 246, are connected to main CPU 232 in power controller 230 via intracontroller bus 240, which may be a RS485 communications link. Smart display 242, smart battery 244 and smart fuel control 246 performs dedicated controller functions, including but not limited to display, energy storage management, and fuel control functions.

Main CPU 232 in power controller 230 is coupled to user port 248 for connection to a computer, workstation, modem or other data terminal equipment which allows for data acquisition and/or remote control. User port 248 may be implemented using a RS232 interface or other compatible interface.

Main CPU 232 in power controller 230 is also coupled to maintenance port 250 for connection to a computer, workstation, modem or other data terminal equipment which allows for remote development, troubleshooting and field upgrades.

Maintenance port 250 may be implemented using a RS232 interface or other compatible interface.

The main CPU processor software communicates data through a TCP/IP stack over intercontroller bus 252, typically an Ethernet 10 Base 2 interface, to gather data and send commands between power controllers (as shown and discussed in detail with respect to FIG. 15). In accordance with the present invention, the main CPU processor software provides seamless operation of multiple paralleled units as a single larger generator system. One unit, the master, arbitrates the bus and sends commands to all units.

Intercontroller bus 254, which may be a RS485 communications link, provides high-speed synchronization of power output signals directly between converter SPs, such as converter SP 236. Although the main CPU software is not responsible for communicating on the intercontroller bus 254, it informs converter SPs, including converter SP 236, when main CPU 232 is selected as the master.

External option port bus 256, which may be a RS485 communications link, allows external devices, including but not limited to power meter equipment and auto disconnect switches, to be connected to generator SP 234.

In operation, main CPU 232 begins execution with a power on self-test when power is applied to the control board. External devices are detected providing information to determine operating modes the system is configured to handle. Power controller 230 waits for a start command by making queries to external devices. Once received, power controller 230 sequences up to begin producing power. As a minimum, main CPU 232 sends commands to external smart devices 242, 244 and 246 to assist with bringing power controller 230 online. If selected as the master, the software may also send commands to initiate the sequencing of other power controllers (FIG. 15) connected in parallel. A stop command will shutdown the system bringing it offline.

System I/O

The main CPU 232 software interfaces with several electronic circuits (not shown) on the control board to operate devices that are universal to all power controllers 230. Interface to system I/O begins with initialization of registers within

power controller 230 to configure internal modes and select external pin control. Once initialized, the software has access to various circuits including discrete inputs/outputs, analog inputs/outputs, and communication ports. These external devices may also have registers within them that require initialization before the device is operational.

- 5 Each of the following sub-sections provides a brief overview that defines the peripheral device the software must interface with. The contents of these sub-sections do not define the precise hardware register initialization required.

Communications

- 10 Referring to FIG. 9, main CPU 232 is responsible for all communication systems in power controller 230. Data transmission between a plurality of power controllers 230 is accomplished through intercontroller bus 252. Main CPU 232 initializes the communications hardware attached to power controller 230 for intercontroller bus 252.

- 15 Main CPU 232 provides control for external devices, including smart devices 242, 244 and 246, which share information to operate. Data transmission to external devices, including smart display 242, smart battery 244 and smart fuel control 246 devices, is accomplished through intracontroller communications bus 240. Main CPU 232 initializes any communications hardware attached to power controller 230 for intracontroller communications bus 240 and implements features defined for the bus master on intracontroller communications bus 240.

- 20 Communications between devices such as switch gear and power meters used for master control functions exchange data across external equipment bus 246. Main CPU 232 initializes any communications hardware attached to power controller 230 for external equipment port 246 and implements features defined for the bus master on external equipment bus 246.

- 25 Communications with a user computer is accomplished through user interface port 248. Main CPU 232 initializes any communications hardware attached to power controller 230 for user interface port 248. In a typical configuration, at power up, the initial baud rate will be selected to 19200 baud, 8 data bits, 1 stop, and no parity. The user has the ability to adjust and save the communications rate setting via user interface port 248 or optional smart external display 242. The saved communications rate is

used the next time power controller 230 is powered on. Main CPU 232 communicates with a modem (not shown), such as a Hayes compatible modem, through user interface port 248. Once communications are established, main CPU 232 operates as if were connected to a local computer and operates as a slave on user interface port 248 (it only responds to commands issued).

Communications to service engineers, maintenance centers, and so forth are accomplished through maintenance interface port 250. Main CPU 232 initializes the communications to any hardware attached to power controller 230 for maintenance interface port 250. In a typical implementation, at power up, the initial baud rate will be selected to 19200 baud, 8 data bits, 1 stop, and no parity. The user has the ability to adjust and save the communications rate setting via user port 248 or optional smart external display 242. The saved communications rate is used the next time power controller 230 is powered on. Main CPU 232 communicates with a modem, such as a Hayes compatible modem, through maintenance interface port 250. Once communications are established, main CPU 232 operates as if it were connected to a local computer and operates as a slave on maintenance interface port 250 (it only responds to commands issued).

Controls

Referring to FIG. 9, main CPU 232 orchestrates operation for motor, converter, and engine controls for power controller 230. The main CPU 232 does not directly perform motor and converter controls. Rather, generator and converter SP processors 234 and 236 perform the specific control algorithms based on data communicated from main CPU 232. Engine controls are performed directly by main CPU 232 (see FIG. 14).

Main CPU 232 issues commands via SPI communications bus 238 to generator SP 234 to execute the required motor control functions. Generator SP 234 will operate the motor (not shown) in either a DC bus mode or a RPM mode as selected by main CPU 232. In the DC bus voltage mode, generator SP 234 uses power from the motor to maintain the DC bus at the setpoint. In the RPM mode, generator SP 234 uses power from the motor to maintain the engine speed at the setpoint. Main CPU 232 provides Setpoint values.

Main CPU 232 issues commands via SPI communications bus 238 to converter SP 236 to execute required converter control functions. Converter SP 236 will operate the converter (not shown) in a DC bus mode, output current mode, or output voltage mode as selected by main CPU 232. In the DC bus voltage mode, converter SP 236 regulates the utility power provided by power controller 230 to maintain the internal bus voltage at the setpoint. In the output current mode, converter SP 236 uses power from the DC bus to provide commanded current out of the converter. In the output voltage mode, converter SP 236 uses power from the DC bus to provide commanded voltage out of the converter. Main CPU 232 provides Setpoint values.

Referring to FIGS. 10-12, control loops 260, 282 and 300 are used to regulate engine controls. These loops include exhaust gas temperature (EGT) control (FIG. 10), speed control (FIG. 11) and power control (FIG. 12). All three of the control loops 260, 282 and 300 are used individually and collectively by main CPU 232 to provide the dynamic control and performance required of power controller 230. These loops are joined together for different modes of operation.

The open-loop light off control algorithm is a programmed command of the fuel device used to inject fuel until combustion begins. In a typical configuration, main CPU 232 takes a snap shot of the engine EGT and begins commanding the fuel device from about 0% to 25% of full command over about 5 seconds. Engine light is declared when the engine EGT rises about 28° C (50° F) from the initial snap shot.

Referring to FIG. 10, EGT control mode loop 260 provides various fuel output commands to regulate the temperature of the turbine. Engine speed signal 262 is used to determine the maximum EGT setpoint temperature 266 in accordance with predetermined setpoint temperature values. EGT setpoint temperature 266 is compared by comparator 268 against feedback EGT signal 270 to determine error signal 272, which is then applied to a proportional-integral (PI) algorithm 274 for determining the fuel command required to regulate EGT at the setpoint. Maximum/minimum fuel limits 278 are used to limit EGT control algorithm fuel command output 276 to protect from integrator windup. Resultant output signal 280 is regulated EGT signal fuel flow command. In operation, EGT control mode loop 260 operates at about a 100 ms rate.

Referring to FIG. 11, speed control mode loop 282 provides various fuel output commands to regulate the rotating speed of the turbine. Feedback speed signal 288 is read and compared by comparator 286 against setpoint speed signal 284 to determine error signal 290, which is then applied to PI algorithm 292 to determine the fuel command required to regulate engine speed at the setpoint. EGT control (FIG. 10) and maximum/minimum fuel limits are used in conjunction with the speed control algorithm 282 to protect output signal 294 from surge and flame out conditions. Resultant output signal 298 is regulated turbine speed fuel flow command. In a typical implementation, speed control mode loop 282 operates at about a 20ms rate.

Referring to FIG. 12, power control mode loop 300 regulates the power producing potential of the turbine. Feedback power signal 306 is read and compared by comparator 304 against setpoint power signal 302 to determine error signal 308, which is then applied to PI algorithm 310 to determine the speed command required to regulate output power at the setpoint. Maximum/minimum speed limits are used to limit the power control algorithm speed command output to protect output signal 312 from running into over speed and under speed conditions. Resultant output signal 316 is regulated power signal turbine speed command. In a typical implementation, the maximum operating speed of the turbine is generally 96,000 RPM and the minimum operating speed of the turbine is generally 45,000 RPM. The loop operates generally at about a 500 ms rate.

Start Only Battery

Referring to FIG. 14, energy storage device 470 may be a start only battery. In the DC bus voltage control mode, start only battery 470 provides energy to regulate voltage to the setpoint command. Main CPU 472 commands the bus voltage to control at different values depending on the configuration of power controller 478. In the state of charge (SOC) control mode, the start only battery system provides a recharging power demand when requested. Available recharging power is generally equivalent to maximum engine power less power being supplied to the output load and system parasitic loads. Main CPU 472 transmits a recharging power level that is the minimum of the original power demand and available recharging power.

Transient Battery

The transient battery provides the DC bus voltage control as described below as well as the state of charge (SOC) control mode described for the start only battery. The transient battery contains a larger energy storage device than the start only battery.

DC Bus Voltage Control

- 5 DC bus 462 supplies power for logic power, external components and system power output. TABLE 1 defines the setpoint the bus voltage is to be controlled at based on the output power configuration of power controller 478:

TABLE 1

10	<u>B3 POWER OUTPUT</u>	<u>SETPOINT</u>
	480/400 VAC Output	800 Vdc
	240/208 VAC Output	400 Vdc

- In the various operating modes, power controller 478 will have different control algorithms responsible for managing the DC bus voltage level. Any of the battery options 470 as well as SPs 456 and 458 have modes that control power flow to regulate the voltage level of DC bus 462. Under any operating circumstances, only one device is commanded to a mode that regulates DC bus 462. Multiple algorithms would require sharing logic that would inevitably make system response slower and software more difficult to comprehend.
- 15
- 20

System States

- Referring to FIG. 13, state diagram 320 showing various operating states of power controller 478 is illustrated. Sequencing the system through the entire operating procedure requires power controller to transition through the operating states defined in
- 25 TABLE 2.

TABLE 2

30	<u>STATE #</u>	<u>SYSTEM STATE</u>	<u>DESCRIPTION</u>
	0	Power Up	Performs activities of initializing and testing the system.
	1	Stand By	Closer power to bus and continues system monitoring

			while waiting for a start command.
2	Prepare to Start	Initializes any external devices preparing for the start procedure.	
3	Bearing	Configures the system and commands the engine to be	
5	Lift Off	rotated to a predetermined RPM, such as 25,000 RPM.	
4	Open Loop Light Off	Turns on ignition system and commands fuel open loop to light the engine.	
5	Closed Loop Acceleration	Continues motoring and closed fuel control until the system reaches the no load state.	
10	6 Run	Engine operates in a no load self-sustaining state producing power only to operate the controller.	
	7 Load	Converter output contactor is closed and system is producing power.	
	8 Re-Charge	System operates off of fuel only and produces power for recharging energy storage device if installed.	
15	9 Cooldown	System is motoring engine to reduce EGT before shutting down.	
	10 Re-Start	Reduces engine speed to begin open loop light when a start command is received in the cooldown state.	
20	11 Re-Light	Performs a turbine re-light in transition from the cooldown to warmdown state. Allows continued engine cooling when motoring is no longer possible.	
	12 Warmdown	Sustains turbine operation with fuel at a predetermined RPM, such as 50,000 RPM, to cool when engine motoring is not possible.	
25	13 Shutdown	Reconfigures the system after a cooldown to enter the stand by state.	
	14 Fault	Turns off all outputs when presence of fault which disables power conversion exists. Logic power is still available for interrogating system faults.	
30	15 Disable	Fault has occurred where processing may no longer	

be possible. All system operation is disabled.

Main CPU 472 begins execution in the "power up" state 322 after power is applied. Transition to the "stand by" state 324 is performed upon successfully completing the tasks of the "power up" state 322. Initiating a start cycle transitions the system to the "prepare to start" state 326 where all system components are initialized for an engine start. The engine then sequences through start states and onto the "run/load" state 328. To shutdown the system, a stop command which sends the system into either "warm down" or "cool down" state 332 is initiated. Systems that have a battery may enter the "re-charge" state 334 prior to entering the "warm down" or "cool down" state 332. When the system has finally completed the "warm down" or "cool down" process 332, a transition through the "shut down" state 330 will be made before the system re-enters the "standby" state 324 awaiting the next start cycle.

During any state, detection of a fault with a system severity level indicating the system should not be operated will transition the system state to "fault" state 334. Detection of faults that indicate a processor failure has occurred will transition the system to the "disable" state 336.

One skilled in the art will recognize that in order to accommodate each mode of operation, the state diagram is multidimensional to provide a unique state for each operating mode. For example, in the "prepare to start" state 326, control requirements will vary depending on the selected operating mode. Therefore, the presence of a stand-alone "prepare to start" state 326, stand-alone transient "prepare to start" state 326, utility grid connect "prepare to start" state 326 and utility grid connect transient "prepare to start" state 326 will be required. Each combination is known as a system configuration (SYSCON) sequence. Main CPU 472 identifies each of the different system configuration sequences in a 16-bit word known as a SYSCON word, which is a bit-wise construction of an operating mode and system state number. In a typical configuration, the system state number is packed in bits 0 through 11. The operating mode number is packed in bits 12 through 15. This packing method provides the system with the capability of sequence through 4096 different system states in 16 different operating modes.

Separate “power up” 322, “re-light” 338, “warm down” 332, “fault” 334 and “disable” 336 states are not required for each mode of operation. The contents of these states are mode independent.

“Power Up” State

- 5 Operation of the system begins in the “power up” state 322 once application of power activates main CPU 472. Once power is applied to power controller 478, all the hardware components will be automatically reset by hardware circuitry. Main CPU 472 is responsible for ensuring the hardware is functioning correctly and configure the components for operation. Main CPU 472 also initializes its own internal data
- 10 structures and begins execution by starting the Real-Time Operating System (RTOS). Successful completion of these tasks directs transition of the software to the “stand by” state 324. Main CPU 472 performs these procedures in the following order:
1. Initialize main CPU 472
 2. Perform RAM Test
 - 15 3. Perform FLASH Checksum
 4. Start RTOS
 5. Run Remaining POST
 6. Initialize SPI Communications
 7. Verify Generator SP Checksum
 - 20 8. Verify Converter SP Checksum
 9. Initialize IntraController Communications
 10. Resolve External Device Addresses
 11. Look at Input Line Voltage
 12. Determine Mode
 - 25 13. Initialize Maintenance Port
 14. Initialize User Port
 15. Initialize External Option Port
 16. Initialize InterController
 17. Chose Master/Co-Master
 - 30 18. Resolve Addressing
 19. Transition to Stand By State (depends on operating mode)

“Stand By” State

Main CPU 472 continues to perform normal system monitoring in the “stand by” state 324 while it waits for a start command signal. Main CPU 472 commands either energy storage device 470 or utility 468 to provide continuous power supply. In operation, main CPU 472 will often be left powered on waiting to be start or for troubleshooting purposes. While main CPU 472 is powered up, the software continues to monitor the system and perform diagnostics in case any failures should occur. All communications will continue to operate providing interface to external sources. A start command will transition the system to the “prepare to start” state 326.

“Prepare to Start” State

Main CPU 472 prepares the control system components for the engine start process. Many external devices may require additional time for hardware initialization before the actual start procedure can commence. The “prepare to start” state 326 provides those devices the necessary time to perform initialization and send acknowledgment to the main CPU 472 that the start process can begin. Once also systems are ready to go, the software shall transition to the “bearing lift off” state 328.

“Bearing Lift Off” State

Main CPU 472 commands generator SP 456 to motor the engine 454 from typically about 0 to 25,000 RPM to accomplish the bearing lift off procedure. A check is performed to ensure the shaft is rotating before transition to the next state occurs.

“Open Loop Light Off” State

Once the motor 452 reaches its liftoff speed, the software commences and ensures combustion is occurring in the turbine. In a typical configuration, main CPU 472 commands generator SP 456 to motor the engine 454 to a dwell speed of about 25,000 RPM. Execution of the open loop light off state 340 starts combustion. Main CPU 472 then verifies that the engine 454 has not met the “fail to light” criteria before transition to the “closed loop accel” state 342.

“Closed Loop Accel” State

Main CPU 472 sequences engine 454 through a combustion heating process to bring the engine 454 to a self-sustaining operating point. In a typical configuration, commands are provided to generator SP 456 commanding an increase in engine speed

to about 45,000 RPM at a rate of about 4000 RPM/sec. Fuel controls are executed to provide combustion and engine heating. When engine 454 reaches "no load" (requires no electrical power to motor), the software transitions to "run" state 344.

"Run" State

5 Main CPU 472 continues operation of control algorithms to operate the engine at no load. Power may be produced from engine 454 for operating control electronics and recharging any energy storage device 470 for starting. No power is output from load converter 458. A power enable signal transitions the software into "load" state 346. A stop command transitions the system to begin shutdown procedures (may vary
10 depending on operating mode).

"Load" State

Main CPU 472 continues operation of control algorithms to operate the engine 454 at the desired load. Load commands are issued through the communications ports, display or system loads. A stop command transitions main CPU 472 to begin
15 shutdown procedures (may vary depending on operating mode). A power disable signal can transition main CPU 472 back to "run" state 344.

"Re-charge" State

Systems that have an energy storage option may be required to charge energy storage device 470 to maximum capacity before entering the "warmdown" 348 or
20 "cooldown" 332 states. During the "re-charge" state 334 of operation, main CPU 472 continues operation of the turbine producing power for battery charging and controller supply. No out power is provided. When the energy storage device 470 has charged, the system transitions to either the "cooldown" 332 or "warmdown" 348 state depending on system fault conditions.

"Cool Down" State

25 "Cool down" state 332 provides the ability to cool the turbine after operation and a means of purging fuel from the combustor. After normal operation, software sequences the system into "cool down" state 332. In a typical configuration, engine 454 is motored to a cool down speed of about 45,000 RPM. Airflow continues to
30 move through engine 454 preventing hot air from migrating to mechanical components in the cold section. This motoring process continues until the engine EGT falls below

a cool down temperature of about 193°C (380°F). Cool down may be entered at much lower than the final cool down temperature when engine 454 fails to light. The engine's combustor requires purging of excess fuel which may remain. The software always operates the cool down cycle for a minimum purge time of 60 seconds. This
 5 purge time ensures remaining fuel is evacuated from the combustor. Completion of this process transitions the system into the "shutdown" state 330. For user convenience, the system does not require a completion of the enter "cooldown" state 332 before being able to attempt a restart. Issuing a start command transitions the system into the "restart" state 350.

10 "Restart" State

Engine 454 is configured from the "cool down" state 332 before engine 454 can be restart. In a typical configuration, the software lowers the engine speed to about 25,000 RPM at a rate of 4,000 RPM/sec. Once the engine speed has reached this level, the software transitions the system into the "open loop light off" state to perform the
 15 actual engine start.

"Shutdown" State

During the "shutdown" state 330, the engine rotor is brought to rest and system outputs are configured for idle operation. In a typical configuration, the software commands the rotor to rest by lowering the engine speed at a rate of 2,000 RPM/sec or
 20 no load condition, whichever is faster. Once the speed reaches about 14,000 RPM, the generator SP is commanded to reduce the shaft speed to about 0 RPM in less than 1 second.

"Re-light" State

When a system fault occurs where no power is provided from the utility or
 25 energy storage device 470, the software re-ignites combustion to perform a warm down. The generator SP is configured to regulate voltage (power) for the internal DC bus. Fuel is added as defined in the open loop light off fuel control algorithm to ensure combustion occurs. Detection of engine light will transition the system to "warm down" state 348.

30 "Warm Down" State

Fuel is provided when no electric power is available to operate engine 454 at a no load condition to lower the operating temperature in “warm down” state 348. In a typical configuration, engine speed is operated at about 50,000 RPM by supplying fuel through the speed control algorithm. Engine temperatures less than about 343°C
 5 (650°F) causes the system to transition to “shutdown” state 330.

“Fault” State

The present invention disables all outputs placing the system in a safe configuration when faults that prohibit safe operation of the turbine system are present. Operation of system monitoring and communications will continue if the energy is
 10 available.

“Disable” State

The system disables all outputs placing the system in a safe configuration when faults that prohibit safe operation of the turbine system are present. System monitoring and communications will most likely not continue.

15 Modes of Operation

The turbine works in two major modes – utility grid-connect and stand-alone. In the utility grid-connect mode, the electric power distribution system i.e., the utility grid, supplies a reference voltage and phase, and the turbine supplies power in synchronism with the utility grid. In the stand-alone mode, the turbine supplies its own
 20 reference voltage and phase, and supplies power directly to the load. The power controller switches automatically between the modes.

Within the two major modes of operation are sub-modes. These modes include stand-alone black start, stand-alone transient, utility grid connect and utility grid connect transient. The criteria for selecting an operating mode is based on numerous
 25 factors, including but not limited to, the presence of voltage on the output terminals, the black start battery option, and the transient battery option.

Referring to FIG. 14, generator converter 456 and load converter 458 provide an interface for energy source 460 and utility 468, respectively, to DC bus 462. For illustrative purposes, energy source 460 is a turbine including engine 454 and generator
 30 452. Fuel device 474 provides fuel via fuel line 476 to engine 454. Generator converter 456 and load converter 458 operate as customized bi-directional switching

converters under the control of controller 472. In particular, controller 472 reconfigures the generator converter 456 and load converter 458 into different configurations to provide for the various modes of operation. These modes include stand-alone black start, stand-alone transient, utility grid connect and utility grid connect transient as discussed in detail below. Controller 472 controls the way in which generator 452 and utility 468 sinks or sources power, and DC bus 462 is regulated at any time. In this way, energy source 460, utility/load 468 and energy storage device 470 can be used to supply, store and/or use power in an efficient manner. Controller 472 provides command signals via line 479 to engine 454 to determine the speed of turbine 460. The speed of turbine 460 is maintained through generator 452. Controller 472 also provides command signals via control line 480 to fuel device 474 to maintain the EGT of the engine 454 at its maximum efficiency point. Generator SP 456 is responsible for maintaining the speed of the turbine 460, but putting current into generator 452 or pulling current out of generator 452.

Stand-alone Black Start

Referring to FIG. 14, in the stand-alone black start mode, energy storage device 470, such as battery, is provided for starting purposes while energy source 460, such as turbine including engine 454 and generator 452, supplies all transient and steady state energy. Referring to TABLE 3, controls for a typical stand-alone black start mode are shown.

TABLE 3

SYSTEM STATE	ENGINE CONTROLS	MOTOR CONTROLS	CONVERTER CONTROLS	ENERGY STORAGE CONTROLS
Power Up	-	-	-	-
Stand By	-	-	-	DC Bus
Prepare to Start	-	-	-	DC Bus
Bearing Lift Off	-	RPM	-	DC Bus
Open Loop Light Off	Open Loop	RPM	-	DC Bus
	Light			
Closed Loop Accel	EGT	RPM	-	DC Bus
Run	Speed	DC Bus	-	SOC
Load	Speed	DC Bus	Voltage	SOC

	Recharge	Speed	DC Bus	-	SOC
	Cool Down	-	RPM	-	DC Bus
	Restart	-	RPM	-	DC Bus
	Shutdown	-	RPM	-	DC Bus
5	Re-light	Speed	DC Bus	-	-
	Warm Down	Speed	DC Bus	-	-
	Fault	-	-	-	-
	Disable	-	-	-	-

10 Stand-alone Transient

In the stand-alone transient mode, storage device 479 is provided for the purpose of starting and assisting the energy source 460, in this example the turbine, to supply maximum rated output power during transient conditions. Storage device 479, typically a battery, is always attached to DC bus 462 during operation, supplying energy in the form of current to maintain the voltage on DC bus 462. Converter/SP 458 provides a constant voltage source when producing output power. As a result, load 468 is always supplied the proper AC voltage value that it requires. Referring to TABLE 4, controls for a typical stand-alone transient mode are shown.

TABLE 4

20	SYSTEM STATE	ENGINE CONTROLS	MOTOR CONTROLS	CONVERTER CONTROLS	ENERGY STORAGE CONTROLS
	Power Up	-	-	-	-
	Stand By	-	-	-	DC Bus
25	Prepare to Start	-	-	-	DC Bus
	Bearing Lift Off	-	RPM	-	DC Bus
	Open Loop Light Off	Open Loop Light	RPM	-	DC Bus
	Closed Loop Accel	EGT	RPM	-	DC Bus
30	Run	Power & EGT	RPM	-	DC Bus
	Load	Power & EGT	RPM	Voltage	DC Bus
	Recharge	Power & EGT	RPM	-	DC Bus
	Cool Down	-	RPM	-	DC Bus
	Restart	-	RPM	-	DC Bus

	Shutdown	-	RPM	-	DC Bus
	Re-light	Speed	DC Bus	-	-
	Warm Down	Speed	DC Bus	-	-
	Fault	-	-	-	-
5	Disable	-	-	-	-

Utility Grid Connect

Referring to FIG. 14, in the utility grid connect mode, the energy source 460, in this example the turbine is connected to the utility grid 468 providing load leveling and management where transients are handled by the utility grid 468. The system operates as a current source, pumping current into utility 468. Referring to TABLE 5, controls for a typical utility grid connect mode are shown.

TABLE 5

	SYSTEM STATE	ENGINE CONTROLS	MOTOR CONTROLS	CONVERTER CONTROLS	ENERGY STORAGE CONTROLS
	Power Up	-	-	-	N/A
	Stand By	-	-	-	N/A
20	Prepare to Start	-	-	DC Bus	N/A
	Bearing Lift Off	-	RPM	DC Bus	N/A
	Open Loop Light Off	Open Loop Light	RPM	DC Bus	N/A
	Closed Loop Accel	EGT	RPM	DC Bus	N/A
25	Run	Power & EGT	RPM	DC Bus	N/A
	Load	Power & EGT	RPM	DC Bus	N/A
	Recharge	N/A	N/A	N/A	N/A
	Cool Down	-	RPM	DC Bus	N/A
	Restart	-	RPM	DC Bus	N/A
30	Shutdown	-	RPM	DC Bus	N/A
	Re-light	Speed	DC Bus	-	N/A
	Warm Down	Speed	DC Bus	-	N/A
	Fault	-	-	-	N/A
	Disable	-	-	-	N/A

Utility Grid Connect Transient

In the utility grid connect transient mode, the energy source 460, in this example the turbine, is connected to the utility grid 468 providing load leveling and management. The turbine that is assisted by energy storage device 470, typically a battery, handles transients. The system operates as a current source, pumping current into utility 468 with the assistance of energy storage device 470. Referring to TABLE 6, controls for a typical utility grid connect transient mode are shown.

10

TABLE 6

	<u>SYSTEM STATE</u>	<u>ENGINE CONTROLS</u>	<u>MOTOR CONTROLS</u>	<u>CONVERTER CONTROLS</u>	<u>ENERGY STORAGE CONTROLS</u>
	Power Up	-	-	-	-
15	Stand By	-	-	-	DC Bus
	Prepare to Start	-	-	-	DC Bus
	Bearing Lift Off	-	RPM	-	DC Bus
	Open Loop Light Off	Open Loop Light	RPM	-	DC Bus
20	Closed Loop Accel	EGT	RPM	-	DC Bus
	Run	Power & EGT	RPM	-	DC Bus
	Load	Power & EGT	RPM	Current	DC Bus
	Recharge	Power & EGT	RPM	-	DC Bus
	Cool Down	-	RPM	-	DC Bus
25	Restart	-	RPM	-	DC Bus
	Shutdown	-	RPM	-	DC Bus
	Re-light	Speed	DC Bus	-	-
	Warm Down	Speed	DC Bus	-	-
	Fault	-	-	-	-
30	Disable	-	-	-	-

Multi-pack Operation

In accordance with the present invention, the power controller can operate in a single or multi-pack configuration. In particular, power controller, in addition to being

a controller for a single turbogenerator, is capable of sequencing multiple systems as well. Referring to FIG. 15, for illustrative purposes, multi-pack system 510 including three power controllers 518, 520 and 522 is shown. The ability to control multiple controllers 518, 520 and 522 is made possible through digital communications interface and control logic contained in each controllers main CPU (not shown).

Two communications busses 530 and 534 are used to create the intercontroller digital communications interface for multi-pack operation. One bus 534 is used for slower data exchange while the other bus 530 generates synchronization packets at a faster rate. In a typical implementation, for example, an IEEE-502.3 bus links each of the controllers 518, 520 and 522 together for slower communications including data acquisition, start, stop, power demand and mode selection functionality. An RS485 bus links each of the systems together providing synchronization of the output power waveforms.

One skilled in the art will recognize that the number of power controllers that can be connected together is not limited to three, but rather any number of controllers can be connected together in a multi-pack configuration. Each power controller 518, 520 and 522 includes its own energy storage device 524, 526 and 528, respectively, such as a battery. In accordance with another embodiment of the invention, power controllers 518, 520 and 522 can all be connected to the same single energy storage device (not shown), typically a very large energy storage device which would be rated too big for an individual turbine. Distribution panel, typically comprised of circuit breakers, provides for distribution of energy.

Multi-pack control logic determines at power up that one controller is the master and the other controllers become slave devices. The master is in charge of handling all user-input commands, initiating all inter-system communications transactions, and dispatching units. While all controllers 518, 520 and 522 contain the functionality to be a master, to alleviate control and bus contention, one controller is designated as the master.

At power up, the individual controllers 518, 520 and 522 determine what external input devices they have connected. When a controller contains a minimum number of input devices it sends a transmission on intercontroller bus 530 claiming to

be master. All controllers 518, 520 and 522 claiming to be a master begin resolving who should be master. Once a master is chosen, an address resolution protocol is executed to assign addresses to each slave system. After choosing the master and assigning slave addresses, multi-pack system 510 can begin operating.

5 A co-master is also selected during the master and address resolution cycle. The job of the co-master is to act like a slave during normal operations. The co-master should receive a constant transmission packet from the master indicating that the master is still operating correctly. When this packet is not received within a safe time period, 20 ms for example, the co-master may immediately become the master and take
10 over master control responsibilities.

Logic in the master configures all slave turbogenerator systems. Slaves are selected to be either utility grid-connect (current source) or standalone (voltage source). A master controller, when selected, will communicate with its output converter logic (converter SP) that this system is a master. The converter SP is then responsible for
15 transmitting packets over the intercontroller bus 530, synchronizing the output waveforms with all slave systems. Transmitted packets will include at least the angle of the output waveform and error-checking information with transmission expected every quarter cycle to one cycle.

Master control logic will dispatch units based on one of three modes of
20 operation: (1) peak shaving, (2) load following, or (3) base load. Peak shaving measures the total power consumption in a building or application using a power meter, and the multi-pack system 510 reduces the utility consumption of a fixed load, thereby reducing the utility rate schedule and increasing the overall economic return of the turbogenerator. Load following is a subset of peak shaving where a power meter
25 measures the total power consumption in a building or application and the multi-pack system 10 reduces the utility consumption to zero load. In base load, the multi-pack system 10 provides a fixed load and the utility supplements the load in a building or application. Each of these control modes require different control strategies to
optimize the total operating efficiency.

30 A minimum number of input devices are typically desired for a system 510 to claim it is a master during the master resolution process. Input devices that are looked

for include a display panel, an active RS232 connection and a power meter connected to the option port. Multi-pack system 510 typically requires a display panel or RS232 connection for receiving user-input commands and power meter for load following or peak shaving.

- 5 In accordance with the present invention, the master control logic dispatches controllers based on operating time. This would involve turning off controllers that have been operating for long periods of time and turning on controllers with less operating time, thereby reducing wear on specific systems.

Utility Grid Analysis and Transient Ride Through

- 10 Referring to FIGS. 16-18, transient handling system 580 for power controller 620 is illustrated. Transient handling system 580 allows power controller 620 to ride through transients which are associated with switching of correction capacitors on utility grid 616 which causes voltage spikes followed by ringing. Transient handling system 580 also allows ride through of other faults, including but not limited to, short
15 circuit faults on utility grid 616, which cleared successfully, cause voltage sags. Transient handling system 580 is particularly effective towards handling transients associated with digital controllers, which generally have a slower current response rate due to A/D conversion sampling. During a transient, a large change in the current can occur in between A/D conversions. The high voltage impulse caused by transients
20 typically causes an over current in digital power controllers.

- As is illustrated in FIG. 17, a graph 590 showing transients typically present on utility grid 616 is shown. The duration of a voltage transient, measured in seconds, is shown on the x-axis and its magnitude, measured in volts, is shown on the y-axis. A capacitor switching transient, such as shown at 592, which is relatively high in
25 magnitude (up to about 200%) and short in duration (somewhere between 1 and 20 milliseconds) could be problematic to operation of a power controller.

- Referring to FIGS. 16-18, changes on utility grid 616 are reflected as changes in the magnitude of the voltage. In particular, the type and seriousness of any fault or event on utility grid 616 can be determined by magnitude estimator 584, which
30 monitors the magnitude and duration of any change on utility grid 616.

In accordance with the present invention, the effect of voltage transients can be minimized by monitoring the current such that when it exceeds a predetermined level, switching is stopped so that the current can decay, thereby preventing the current from exceeding its predetermined level. The present invention thus takes advantage of analog over current detection circuits that have a faster response than transient detection based on digital sampling of current and voltage. Longer duration transients indicate abnormal utility grid conditions. These must be detected so power controller 620 can shut down in a safe manner. In accordance with the present invention, algorithms used to operate power controller 620 provide protection against islanding of power controller 620 in the absence of utility-supplied grid voltage. Near short or near open islands are detected within milliseconds through loss of current control. Islands whose load is more closely matched to the power controller output will be detected through abnormal voltage magnitudes and frequencies as detected by magnitude estimator 584.

In particular, referring to FIG. 18, power controller 620 includes brake resistor 612 connected across DC bus 622. Brake resistor 612 acts as a resistive load, absorbing energy when converter SP 608 is turned off. In operation, when converter SP 608 is turned off, power is no longer exchanged with utility grid 616, but power is still being received from the turbine, which is absorbed by brake resistor 612. The present invention detects the DC voltage between generator and converter SPs 606 and 608. When the voltage starts to rise, brake resistor 612 is turned on to allow it to absorb energy.

In a typical configuration, AC motor 618 produces three phases of AC at variable frequencies. AC/DC converter 602 under the control of motor SP 606 converts the AC to DC which is then applied to DC bus 622 (regulated for example at 800 vDC) which is supported by capacitor 610 (for example, at 800 microfarads with two milliseconds of energy storage). AC/DC converter 604, under the control of converter SP 608, converts the DC into three-phase AC, and applies it to utility grid 616. In accordance with the present invention, current from DC bus 622 can be dissipated in brake resistor 612 via modulation of switch 614 operating under the control of motor SP 606. Switch 614 may be an IGBT switch, although one skilled in

the art will recognize that other conventional or newly developed switches may be utilized as well.

Motor SP 606 controls switch 614 in accordance to the magnitude of the voltage on DC bus 622. The bus voltage of DC bus 622 is typically maintained by converter SP 608, which shuttles power in and out of utility grid 616 to keep DC bus 622 regulated at, for example, 800 vDC. When converter SP 608 is turned off, it no longer is able to maintain the voltage of DC bus 622, so power coming in from the motor causes bus voltage of DC bus 622 to rise quickly. The rise in voltage is detected by motor SP 606, which turns on brake resistor 612 and modulates it on and off until the bus voltage is restored to its desired voltage, for example, 800 vDC. Converter SP 608 detects when the utility grid transient has dissipated, i.e., AC current has decayed to zero and restarts the converter side of power controller 620. Brake resistor 612 is sized so that it can ride through the transient and the time taken to restart converter.

Referring to FIGS. 18 and 20, in accordance with the present invention, both the voltage and zero crossings (to determine where the AC waveform of utility grid 616 crosses zero) are monitored to provide an accurate model of utility grid 616. Utility grid analysis system includes angle estimator 582, magnitude estimator 584 and phase locked loop 586. The present invention continuously monitors utility grid voltage and based on these measurements, estimates the utility grid angle, thus facilitating recognition of under/over voltages and sudden transients. Current limits are set to disable DC/AC converter 604 when current exceeds a maximum and wait until current decays to an acceptable level. The result of measuring the current and cutting it off is to allow DC/AC converter 604 to ride through transients better. Thus when DC/AC converter 608 is no longer exchanging power with utility grid 616, power is dissipated in brake resistor 612.

In accordance with the present invention, converter SP 608 is capable of monitoring the voltage and current at utility grid 616 simultaneously. In particular, power controller 620 includes a utility grid analysis algorithm. One skilled in the art will recognize that estimates of the utility grid angle and magnitude may be derived via conventional algorithms or means. The true utility grid angle θ_{AC} , which is the angle

of the generating source, cycles through from 0 to 2π and back to 0 at a rate of 60 hertz. The voltage magnitude estimates of the three phases are designated $V_{1\text{ mag}}$, $V_{2\text{ mag}}$ and $V_{3\text{ mag}}$ and the voltage measurement of the three phases are designated V_1 , V_2 and V_3 .

5 A waveform, constructed based upon the estimates of the magnitude and angle for each phase, indicates what a correct measurement would look like. For example, using the first of the three phase voltages, the cosine of the true utility grid angle θ_{AC} is multiplied by the voltage magnitude estimate $V_{1\text{ mag}}$, with the product being a cosine-like waveform. Ideally, the product would be voltage measurement V_1 .

10 Feedback loop 588 uses the difference between the absolute magnitude of the measurement of V_1 and of the constructed waveform to adjust the magnitude of the magnitude estimate $V_{1\text{ mag}}$. One skilled in the art will recognize that the other two phases of three-phase signal can be adjusted similarly, with different angle templates corresponding to different phases of the signal. Thus, magnitude estimate $V_{1\text{ mag}}$ and
15 angle estimate θ_{EST} are used to update magnitude estimate $V_{1\text{ mag}}$. Voltage magnitude estimates $V_{1\text{ mag}}$, $V_{2\text{ mag}}$ and $V_{3\text{ mag}}$ are steady state values used in a feedback configuration to track the magnitude of voltage measurements V_1 , V_2 and V_3 . By dividing the measured voltages V_1 by the estimates of the magnitude $V_{1\text{ mag}}$, the cosine of the angle for the first phase can be determined (similarly, the cosine of the angles of
20 the other signals will be similarly determined).

In accordance with the present invention, the most advantageous estimate for the cosine of the angle, generally the one that is changing the most rapidly, is chosen to determine the instantaneous measured angle. In most cases, the phase that has an estimate for the cosine of an angle closest to zero is selected since it yields the greatest
25 accuracy. Utility grid analysis system 580 thus includes logic to select which one of the cosines to use. The angle chosen is applied to angle estimator 582, from which an estimate of the instantaneous angle θ_{EST} of utility grid 616 is calculated and applied to phase locked loop 586 to produce a filtered frequency. The angle is thus differentiated to form a frequency that is then passed through a low pass filter (not shown). Phase
30 locked loop 586 integrates the frequency and also locks the phase of the estimated

instantaneous angle θ_{EST} , which may have changed in phase due to differentiation and integration, to the phase of true utility grid angle θ_{AC} .

In a typical operation, when the phase changes suddenly on measured voltage V_1 , the algorithm of the present invention compares the product of the magnitude estimate $V_{1\ mag}$ and the cosine of true utility grid angle θ_{AC} against the real magnitude multiplied by the cosine of a different angle. A sudden jump in magnitude would be realized.

Thus, three reasonably constant DC voltage magnitude estimates are generated. A change in one of those voltages indicates whether the transient present on utility grid is substantial or not. One skilled in the art will recognize that there are a number of ways to determine whether a transient is substantial or not, i.e. whether abnormal conditions exist on the utility grid system, which require power controller 620 to shut down. A transient can be deemed substantial based upon the size of the voltage magnitude and duration. Examples of the criteria for shutting down power controller 620 are shown in FIG. 17. Detection of abnormal utility grid behavior can also be determined by examining the frequency estimate.

On detecting abnormal utility grid behavior, a utility grid fault shutdown is initiated. When system controller 620 initiates a utility grid fault shutdown, output contactor is opened within a predetermined period of time, for example, 100 msec, and the main fuel trip solenoid (not shown) is closed, removing fuel from the turbogenerator. A warm shutdown ensues during which control power is supplied from generator 618 as it slows down. In a typical configuration, the warm-down lasts about 1-2 minutes before the rotor (not shown) is stopped. The control software does not allow a restart until utility grid voltage and frequency are within permitted limits.

Having now described the invention in accordance with the requirements of the patent statutes, those skilled in this art will understand how to make changes and modifications in the present invention to meet their specific requirements or conditions. For example, the power controller, while described generally, may be implemented in an analog or digital configuration. In the preferred digital configuration, one skilled in the art will recognize that various terms utilized in the invention are generic to both analog and digital configurations of power controller. For example, converters

referenced in the present application is a general term which includes inverters, signal processors referenced in the present application is a general term which includes digital signal processors, and so forth. Correspondingly, in a digital implementation of the present invention, inverters and digital signal processors would be utilized. Such

5 changes and modifications may be made without departing from the scope and spirit of the invention as set forth in the following claims.

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ABSTRACT OF THE DISCLOSURE**POWER CONTROLLER**

A power controller provides a distributed generation power networking system in which bi-directional power converters are used with a common DC bus for permitting compatibility between various energy components. Each power converter operates essentially as a customized bi-directional switching converter configured, under the control of the power controller, to provide an interface for a specific energy component to the DC bus. The power controller controls the way in which each energy component, at any moment, will sink or source power, and the manner in which the DC bus is regulated. In this way, various energy components can be used to supply, store and/or use power in an efficient manner. The various energy components include energy sources, loads, storage devices and combinations thereof.

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WHAT IS CLAIMED IS:

- 1 1. A power controller for distributing power among a plurality of energy
2 components, comprising:
3 a DC bus; and
4 a plurality of power converters, each of which is connected between one of said
5 energy components and said DC bus and is responsive to said power controller, wherein
6 said power controller provides a distributed generation power system by controlling the
7 way each energy component sinks or sources power and said DC bus is regulated.
- 1 2. A power controller claimed in claim 1, wherein each of said power converters
2 operates as a customized bi-directional switching converter configured, under the control
3 of said power controller, to provide an interface for said energy component to said DC
4 bus.
- 1 3. The power controller claimed in claim 1, wherein each of said power converters
2 comprises:
3 a power switching system; and
4 a processing system for providing control to said power switching system.
- 1 4. The power controller claimed in claim 3, wherein said processing system further
2 comprises:
3 a signal processor; and
4 a central processing unit for providing control to said signal processor.
- 1 5. The power controller claimed in claim 3, wherein said central processing unit
2 reconfigures said power converter into different configurations for different modes of
3 operation.
- 1 6. The power controller claimed in claim 3, wherein said power switching system
2 comprises a plurality of insulated gate bipolar transistor switches.
- 1 7. The power controller claimed in claim 1, wherein said plurality of energy
2 components includes an energy source.

1 8. The power controller claimed in claim 7, wherein said energy source comprises a
2 gas turbine.

1 9. The power controller claimed in claim 8, wherein said gas turbine drives an AC
2 generator to produce AC which is applied to said power converter.

1 10. The power controller claimed in claim 9, wherein said controller regulates DC bus
2 voltage independently of turbine speed.

1 11. The power controller claimed in claim 1, wherein said plurality of energy
2 components includes an energy storage device.

1 12. The power controller claimed in claim 11, wherein said energy storage device
2 comprises a flywheel.

1 13. The power controller claimed in claim 11, wherein said energy storage device
2 comprises a battery.

1 14. The power controller claimed in claim 11, wherein said energy storage device
2 comprises an ultracap.

1 15. The power controller claimed in claim 1, wherein said plurality of energy
2 components includes a load.

1 16. The power controller claimed in claim 15, wherein said load comprises an AC
2 utility.

1 17. The power controller claimed in claim 16, wherein said load comprises a DC
2 load.

1 18. The power controller claimed in claim 16, wherein said load comprises a drive
2 motor.

1 19. The power controller claimed in claim 1, wherein said plurality of energy
2 components includes an energy source, a load and a storage device.

1 20. The power controller claimed in claim 19, wherein during a utility start up mode
2 of operation, one of said power converters applies power from said load to said DC bus
3 for conversion by another of said power converters into power required by said energy
4 source to startup and said storage device is disconnected from said DC bus while said
5 load regulates DC voltage on said DC bus.

1 21. The power controller claimed in claim 20, wherein said energy source comprises
2 a turbine and is controlled in a local feedback loop to maintain said turbine revolutions
3 per minute (RPM).

1 22. The power controller claimed in claim 19, wherein during a utility start up mode
2 of operation, one of said power converters isolates said DC bus so that another of said
3 power converters provides the required starting power from said DC bus to said energy
4 source.

1 23. The power controller claimed in claim 1, wherein said power converters comprise
2 a generator converter and output converter.

1 24. The power controller claimed in claim 23, wherein said power controller is
2 digital, said generator converter is a generator inverter and said output converter is an
3 output inverter.

1 25. The power controller claimed in claim 4, wherein said central processing unit
2 sequences events which occur inside said power controller and arbitrates communications
3 to externally connected devices.

1 26. The power controller claimed in claim 4, wherein said central processing unit is a
2 Motorola MC68332 microprocessor.

1 27. The power controller claimed in claim 19, wherein said energy source comprises
2 a turbogenerator, said energy storage device comprises a battery and said load comprises
3 a utility grid.

1 28. The power controller claimed in claim 19, wherein said energy source comprises
2 a turbogenerator, said energy storage device comprises a capacitive device and said load
3 comprises a utility grid.

1 29. The power controller claimed in claim 19 wherein said energy source comprises a
2 turbogenerator, and said load comprises a utility grid.

1 30. The power controller claimed in claim 1, wherein said plurality of energy
2 components comprises a turbogenerator and a load.

1 31. A turbine system, comprising:
2 a turbine engine;
3 a load; and
4 a power controller for converting electricity from said turbine engine into
5 regulated DC and then to AC electricity, wherein said power controller includes an
6 engine power conversion in communication with said turbine engine, an utility power
7 conversion in communication with said load and a DC bus.

1 32. The turbine system claimed in claim 31, further comprising:
2 a fuel metering system in communication with an energy reservoir controller and
3 said power controller.

1 33. The turbine system claimed in claim 31, wherein said power controller provides a
2 distributed generation power system utilizing said engine power conversion and said
3 utility power conversion.

1 34. The turbine system claimed in claim 31, wherein said engine power conversion
2 and said utility power conversion operate as a customized bi-directional switching
3 converters, under control of said power controller, to provide an interface for said turbine
4 engine and said load to said DC bus.

1 35. A method for controlling the distribution of power among a plurality of energy
2 components, comprising the steps of:
3 connecting a power converter between a DC bus and each of said energy
4 components;
5 controlling the way each of said energy components sinks or sources power; and
6 controlling the way said DC bus is regulated responsive to operation of each of
7 said energy components.

1 36. The method claimed in claim 35, wherein said step of controlling the way each of
2 said energy components sinks or sources power, further comprises the step of:
3 controlling the way each of said power converters is configured.

1 37. The method claimed in claim 35, wherein said step of controlling the way each of
2 said energy components sinks or sources power, further comprises the step of:

controlling said power converters such that they operate as customized, bi-directional switching converters configured to provide an interface for said energy components to said DC bus.

38. The method claimed in claim 36, wherein said each of said power converters comprises a power switching system and said step of controlling the way each of said power converters is configured, further comprises the step of:
providing control to said power switching system.

39. The method claimed in claim 35, wherein said step of controlling the way each of said power converters is configured, further comprises the step of:
reconfiguring said each of said power converters into different configurations for different modes of operation.

40. The method claimed in 35, wherein said plurality of energy components include an energy source, a load and a storage device.

41. The method claimed in claim 40, wherein said energy source comprises a turbogenerator, said energy storage device comprises a battery and said load comprises a utility grid.

42. The method claimed in claim 40, wherein said energy source comprises a turbogenerator, said energy storage device comprises a capacitive device and said load comprises a utility grid.

43. The method claimed in claim 40, further comprising the steps of:
during a utility start up mode of operation, utilizing one of said power converters to apply power from said load to said DC bus for conversion by another of said power converters into power required by said energy source to startup;

disconnecting said storage device from said DC bus while said load regulates DC voltage on said DC bus.

44. The method claimed in claim 43, wherein said energy source comprises a turbine and further comprising the step of:

utilizing a local feedback loop to maintain said revolutions per minute (RPM) of said turbine.

45. The method claimed in claim 40 further comprising the steps of:

2 during a utility start up mode of operation, isolating one of said power converters
3 from said DC bus so that another of said power converters provides the required starting
4 power from said DC bus to said energy source.

1 46. The method claimed in claim 35, wherein said power converters comprise a
2 generator converter and output converter.

1 47. The method claimed in claim 46, wherein said distribution of power is controlled
2 digitally, said generator converter is a generator inverter and said output converter is an
3 output inverter.

1 48. The method claimed in claim 35, further comprising the steps of:
2 sequencing events which occur; and
3 arbitrating communications to externally connected devices.

1 49. A power control system, comprising:
2 a plurality of power controllers for distributing power among a plurality of energy
3 components; and

4 a first bus for providing communication between said plurality of power
5 controllers.

1 50. The power control system claimed in claim 49, further comprising:
2 a second bus for providing communication between said plurality of power
3 controllers.

1 51. The power control system claimed in claim 50, wherein said first bus provides for
2 data exchange at a first rate and said second bus provides for data exchange at a second
3 rate.

1 52. The power control system claimed in claim 51, wherein said first bus provides for
2 synchronization of output power waveforms.

1 53. The power control system claimed in claim 52, wherein said second bus provides
2 for data acquisition.

1 54. The power control system claimed in claim 52, wherein said second bus provides
2 for start and stop operation of said system.

1 55. The power control system claimed in claim 52, wherein said second bus provides
2 mode selection.

- 1 56. The power control system claimed in claim 49, wherein each of said plurality of
2 power controllers comprises:
3 a DC bus; and
4 a plurality of power converters, one of said plurality of power converters
5 connected between one of said plurality of energy components and said DC bus and is
6 responsive to said power controller, wherein said power controller provides a distributed
7 generation power system by controlling the way each energy component sinks or sources
8 power and said DC bus is regulated.
- 1 57. The power control system claimed in claim 52, wherein each of said power
2 converters operates as a customized bi-directional switching converter configured, under
3 the control of said power controller, to provide an interface for said energy component to
4 said DC bus.
- 1 58. The power control system claimed in claim 49, wherein said plurality of power
2 controllers includes a master controller with remainder of said plurality of power
3 controllers being slave controllers..
- 1 59. The power control system claimed in claim 58, wherein said master controller
2 handles user-input commands.
- 1 60. The power control system claimed in claim 58, wherein said master controller
2 initiates inter-system communication transactions.
- 1 61. The power control system claimed in claim 58, wherein said master controller
2 dispatches said slave controllers.
- 1 62. The power control system claimed 58, wherein said system determines a master
2 controller and assigns addresses to said slave controllers.
- 1 63. The power control system claimed in claim 58, wherein said slave controllers
2 includes a co-master controller for monitoring operation of said master controller.
- 1 64. The power control system claimed in claim 63, wherein said co-master controller
2 receives a signal from said master controller indicating that said master controller is
3 operating correctly.
- 1 65. The power control system claimed in claim 58, wherein said slave controllers are
2 selected to be either a current source or standalon

1 66. The power control system claimed in 58, wherein said master controller further
2 comprises:

3 a signal processor; and

4 a central processing unit for providing control to said signal processor.

1 67. The power control system claimed in claim 58, wherein said signal processor is
2 digital.

1 68. The power control system claimed in claim 66, wherein said master controller
2 communicates with said signal processor that it is a master controller.

1 69. The power control system claimed in claim 66, wherein said signal processor
2 transmits packets over said first bus for synchronizing output waveforms with said slave
3 controllers.

1 70. The power control system claimed in claim 69, wherein said packets include an
2 angle of said output waveforms.

1 71. The power control system claimed in claim 69, wherein said packets include
2 error-checking information.

1 72. The power control system claimed in claim 58, wherein said master controller
2 measures total power consumption and said system, in response to said measurement,
3 adjusts utility consumption to a fixed load.

1 73. The power control system claimed in claim 59, wherein said master controller
2 adjusts utility consumption to a zero load.

1 74. The power control system claimed in claim 58, wherein said system provides a
2 fixed load and utility supplements said load in an application.

1 75. The power control system claimed in claim 58, wherein said master controller
2 dispatches slave controllers based on operating time.

1 76. The power control system claimed in claim 75, wherein said master controller
2 turns off slave controllers that have been operating for long periods of time and turning
3 on slave controllers with less operating time by reducing wear on specific slave
4 controllers.

1 77. The power control system claimed in claim 49, wherein system provides for
2 multi-turbogenerator control.

1 78. The power control system claimed in claim 77, further comprising:

2 a plurality of turbine engines;
3 a plurality of loads;
4 wherein said plurality of power controllers convert electricity from said plurality
5 of turbine engines into regulated DC and then to AC electricity, wherein said plurality of
6 power controllers include an engine power conversion in communication with said
7 plurality of turbine engine, an utility power conversion in communication with said
8 plurality of loads and a DC bus.

1 79. A digital power controller for distributing power among a plurality of energy
2 components, comprising:

3 a DC bus; and

4 a plurality of power inverters, each of which is connected between said energy
5 component and said DC bus and is responsive to said power controller, wherein said
6 power controller provides a distributed generation power system by controlling the way
7 each energy component sinks or sources power and said DC bus is regulated,

8 wherein said energy components include an energy source, energy storage device
9 and load.

1 80. The digital power controller claimed in claim 79, wherein said controller operates
2 in a first and second mode.

1 81. The digital power controller claimed in claim 80, wherein in said first mode, said
2 load supplies a reference voltage and phase, and said energy source supplies power in
3 synchronism with said load.

1 82. The digital power controller claimed in claim 80, wherein in said second mode,
2 said energy source supplies its own reference voltage and phase, and supplies power
3 directly to said load.

1 83. The digital power controller claimed in claim 79, wherein said energy source
2 comprises a turbine and said load comprises a grid.

1 84. The digital power controller claimed in claim 80, wherein said controller switches
2 automatically between said first and second modes.

1 85. The digital power controller claimed in claim 80, wherein each of said first and
2 second modes comprises a plurality of sub-modes.

- 1 86. The digital power controller claimed in claim 85, wherein in a first sub-mode,
2 said energy storage device provides for starting and said energy source supplies transient
3 and steady state energy.
- 1 87. The digital power controller claimed in claim 85, wherein in a second sub-mode,
2 said storage device starts and assists said energy source to supply maximum output power
3 during transient conditions.
- 1 88. The digital power controller claimed in claim 87, wherein said storage device is
2 always attached to said DC bus during operation, supplying energy to maintain voltage
3 on said DC bus.
- 1 89. The digital power controller claimed in claim 85, wherein in a third sub-mode,
2 said energy source is connected to said load providing load leveling and management and
3 said load handles transients.
- 1 90. The digital power controller claimed in claim 85, wherein in a fourth sub-mode,
2 said energy source is connected to said load providing load leveling and management and
3 said energy storage device handles transients.
- 1 91. A method of controlling the distribution of power among a plurality of energy
2 components using a computer including a digital signal processor comprising the steps
3 of:
4 interfacing a plurality of power inverters between a DC bus and each of said
5 energy components;
6 controlling the way each of said energy components sinks or sources power; and
7 controlling the way said DC bus is regulated responsive to operation of each of
8 said energy components, wherein said energy components include an energy source, a
9 load and a storage device.
- 1 92. The method claimed in claim 91, further comprising the steps of:
2 applying power to said power inverters for start up;
3 error checking said power inverters;
4 initializing internal data structures; and
5 starting operating system.
- 1 93. The method claimed in claim 92, further comprising the steps of:
2 monitoring said system and performing diagnostics should failures occur; and

3 commanding either energy storage device or load to provide continuous power
4 supply.

1 94. The method claimed in claim 93, further comprising the steps of:
2 initializing external devices; and
3 acknowledging start process can begin.

1 95. The method claimed in claim 94, further comprising the steps of:
2 commanding signal processor to motor said energy source; and
3 ensuring said energy source is rotating.

1 96. The method claimed in claim 95, further comprising the step of:
2 once said energy source reaches a predetermined speed, ensuring combustion is
3 occurring.

1 97. The method claimed in claim 96, further comprising the step of:
2 sequencing said energy source through a heating process to bring said energy
3 source to a self-sustaining operating point.

1 98. The method claimed in claim 97, further comprising the step of:
2 continuing operation of control algorithms to operate said energy source at no
3 load.

1 99. The method claimed in claim 98, further comprising the step of:
2 continuing operation of control algorithms to operate said energy source at a
3 desired load.

1 100. The method claimed in claim 99, further comprising the step of:
2 charging energy storage device to maximum capacity.

1 101. The method claimed in claim 100, further comprising the steps of:
2 cooling said energy source after operation; and
3 purging fuel.

1 102. The method claimed in claim 101, further comprising the step of:
2 configuring said energy source before said energy source is restarted.

1 103. The method claimed in claim 102, further comprising the steps of:
2 resting said energy source; and
3 configuring system outputs for idle operation.

- 1 104. The method claimed in claim 102, further comprising the step of:
2 re-igniting combustion to perform a warm down when a system fault occurs
3 where no power is provided from load or energy storage device.
- 1 105. The method claimed in claim 104, further comprising the step of:
2 providing fuel when no electric power is available to operate said energy source at
3 a no load condition to lower operating temperature in warm down state.
- 1 106. The method claimed in claim 105, further comprising the step of:
2 monitoring said system for faults.
- 1 107. The method claimed in claim 106, further comprising the step of:
2 disabling all outputs so that said system is placed in a safe configuration when
3 faults that prohibit safe operation occur.
- 1 108. A method of controlling the distribution of power in a system including a turbine,
2 among a plurality of energy components, using a computer including a digital signal
3 processor comprising the steps of:
4 interfacing a plurality of power inverters between a DC bus and each of said
5 energy components;
6 controlling the way each of said energy components sinks or sources power; and
7 controlling the way said DC bus is regulated responsive to operation of each of
8 said energy components, wherein said energy components include an energy source, a
9 load and a energy storage device.
- 1 109. The method claimed in claim 108, further comprising the step of:
2 varying a speed command to regulate power of said system.
- 1 110. The method claimed in claim 108, further comprising the step of:
2 varying a fuel flow command to regulate speed of said turbine.
- 1 111. The method claimed in claim 108, further comprising the step of:
2 varying a fuel flow command to regulate exhaust gas temperature of said turbine.
- 1 112. The method claimed in claim 108, wherein said power inverters include first and
2 second power inverters under the control of first and second signal processors,
3 respectively.
- 1 113. The method claimed in claim 112, further comprising the step of:

2 varying a current command associated with said first signal processor to regulate
3 a speed of said turbine.

1 114. The method claimed in claim 112, further comprising the step of:

2 varying a current command associated with said second signal processor to
3 regulate voltage of said DC bus.

1 115. The method claimed in claim 112, further comprising the step of:

2 varying a current command associated with said first signal processor to regulate
3 voltage of said DC bus.

1 116. The method claimed in claim 112, further comprising the step of:

2 providing power from said DC bus in accordance with said second signal
3 processor to provide a constant AC voltage output.

1 117. The method claimed in claim 108, further comprising the step of:

2 providing power bi-directionally from said energy storage device to regulate
3 voltage of said DC bus.

1 118. The method claimed in claim 108, further comprising the step of:

2 providing power from said DC bus in accordance with said second signal
3 processor to provide a constant AC current output.

1 119. The method claimed in claim 108, further comprising the step of:

2 varying an AC current command to said second signal processor to regulate a
3 constant turbine EGT.

1 120. The method claimed in claim 108, further comprising the step of:

2 providing power bi-directionally from said energy storage device to regulate a device
3 state of charge.

1 121. A method of controlling the distribution of power in a system including a turbine,
2 among a plurality of energy components, using a computer including a digital signal
3 processor comprising the steps of:

4 interfacing a plurality of power inverters between a DC bus and each of said
5 energy components;

6 controlling the way each of said energy components sinks or sources power; and

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2 varying an AC current command to said second signal processor to regulate a
3 constant turbine EGT.

1 133. The method claimed in claim 132, further comprising the step of:
2 providing power bi-directionally from said energy storage device to regulate a device
3 state of charge.

1 134. A power controller for distributing power among a plurality of energy
2 components, comprising:

3 a DC bus;

4 a plurality of power converters, each of which is connected between one of said
5 energy components and said DC bus and is responsive to said power controller, wherein
6 said power controller provides a distributed generation power system by controlling the
7 way each energy component sinks or sources power and said DC bus is regulated; and

8 means for detecting transients associated with one of said energy components.

1 135. The power controller claimed in claim 134, further comprising:

2 means for suspending power transfer between one of said energy components and
3 one of said power converters.

1 136. The power controller claimed in claim 135, further comprising:

2 means for resuming power transfer between one of said energy components and
3 one of said power converters once current in said one of said energy components has
4 decayed to near zero.

1 137. The power controller claimed in claim 136, further comprising:

2 means for dissipating via a resistive load said power fed into said DC bus by said
3 other one of said energy components.

1 138. The power controller claimed in claim 134, further comprising:

2 means for estimating phase voltage magnitudes and grid phase angle in a
3 feedback process, in conjunction with measurements of actual phase voltages to improve
4 estimated peak voltage magnitudes;

5 means for estimating an instantaneous angle of each phase of an utility grid based
6 on said estimated peak voltage magnitudes and measured phase voltages;

7 means for utilizing most accurate angle estimate to calculate an estimate of an
8 instantaneous phase angle of said grid;

9 means for differentiating and filtering to form an estimate of grid frequency;
 10 means for integrating said grid frequency to produce an estimated grid phase
 11 angle; and
 12 means for correcting said estimated grid phase angle to converge in phase with an
 13 estimate of an instantaneous phase angle of said grid.

1 139. A method for controlling the distribution of power among a plurality of energy
 2 components, comprising the steps of:

3 connecting a power converter between a DC bus and each of said energy
 4 components;
 5 controlling the way each of said energy components sinks or sources power;
 6 controlling the way said DC bus is regulated responsive to operation of each of
 7 said energy components; and
 8 detecting transients associated with one of said energy components.

1 140. The method claimed in claim 139, further comprising the step of:
 2 suspending power transfer between one of said energy components and one of
 3 said power converters.

1 141. The method claimed in claim 140, further comprising the step of:
 2 resuming power transfer between one of said energy components and one of said
 3 power converters once current in said one of said energy components has decayed to near
 4 zero.

1 142. The method claimed in claim 141, further comprising the step of:
 2 dissipating via a resistive load said power fed into said DC bus by said other one
 3 of said energy components.

1 143. The method claimed in claim 139, further comprising the steps of:
 2 estimating phase voltage magnitudes and grid phase angle in a feedback process,
 3 in conjunction with measurements of actual phase voltages to improve estimated peak
 4 voltage magnitudes;
 5 estimating an instantaneous angle of each phase of an utility grid based on said
 6 estimated peak voltage magnitudes and measured phase voltages;
 7 utilizing most accurate angle estimate to calculate an estimate of an instantaneous
 8 phase angle of said grid;

- 9 differentiating and filtering to form an estimate of grid frequency;
- 10 means for integrating said grid frequency to produce an estimated grid phase
- 11 angle; and
- 12 correcting said estimated grid phase angle to converge in phase with an estimate
- 13 of an instantaneous phase angle of said grid.

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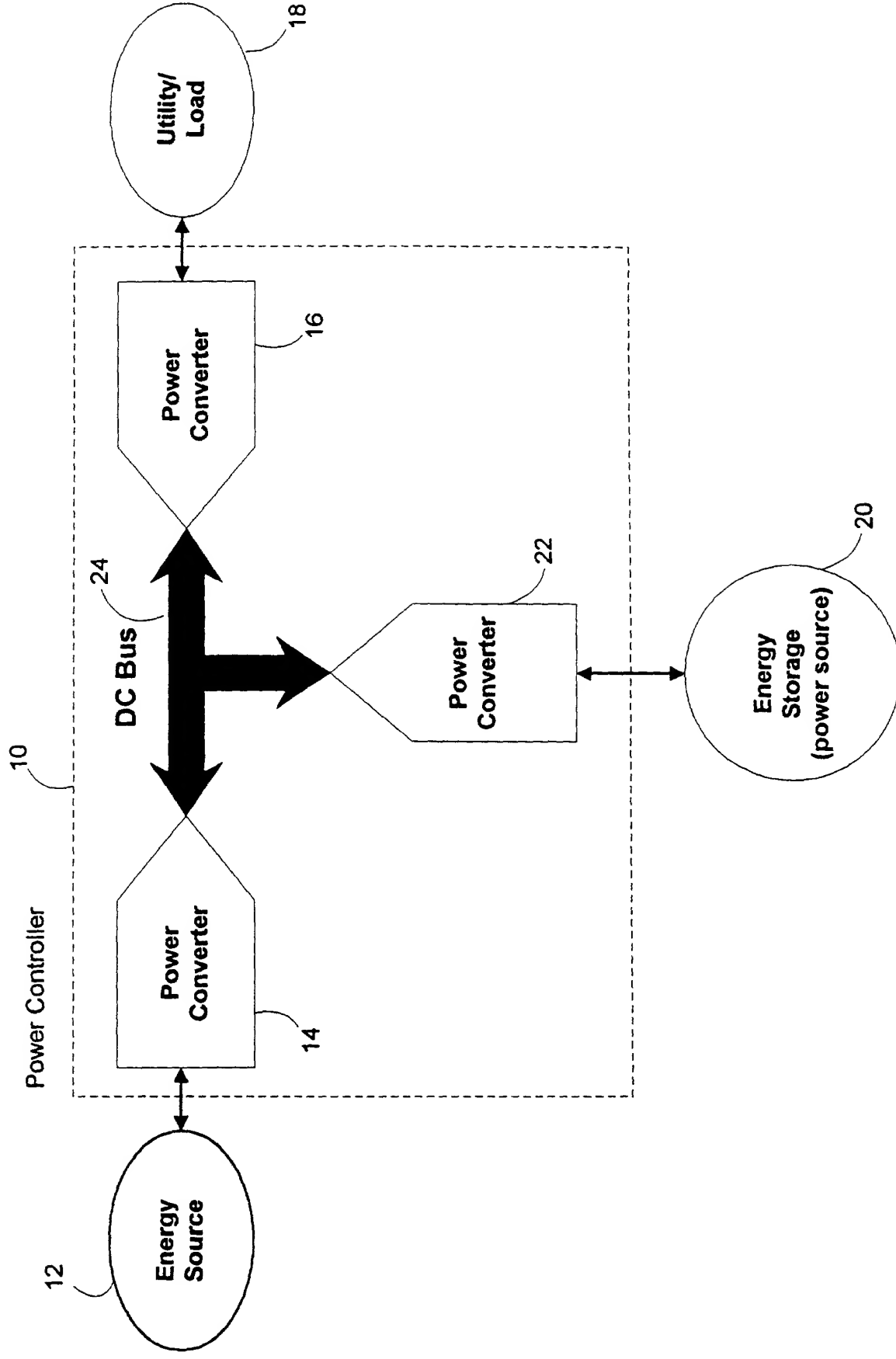


FIG. 1

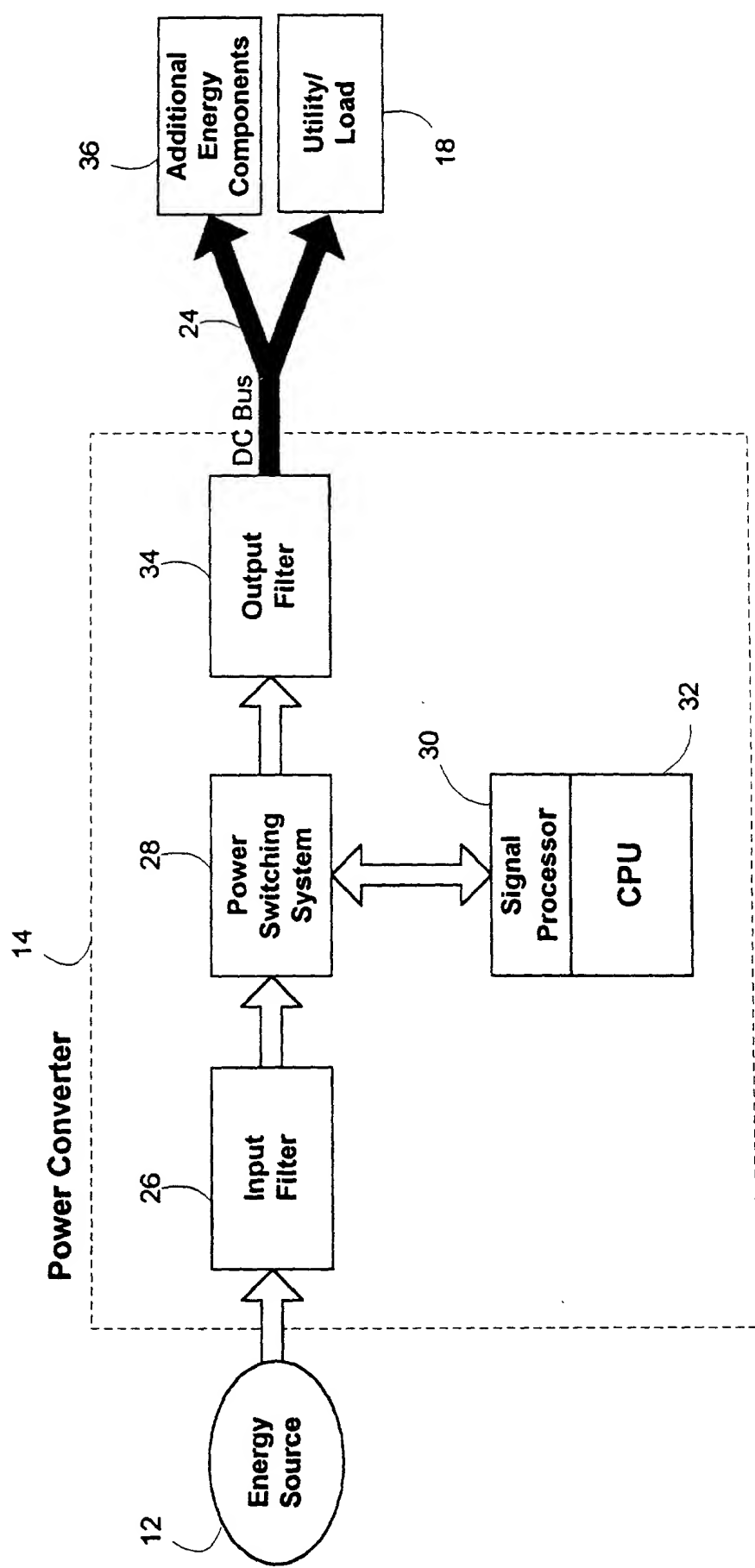
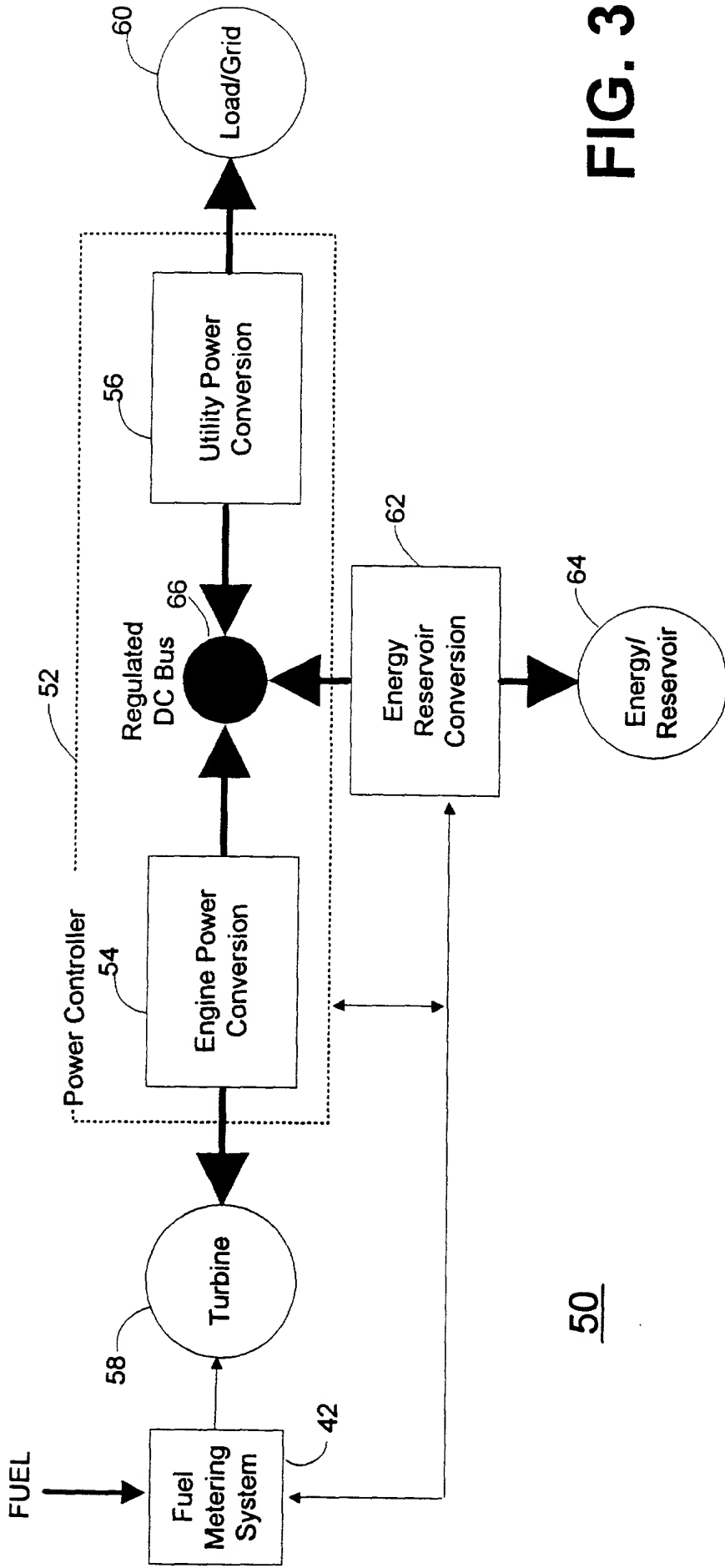


FIG. 2



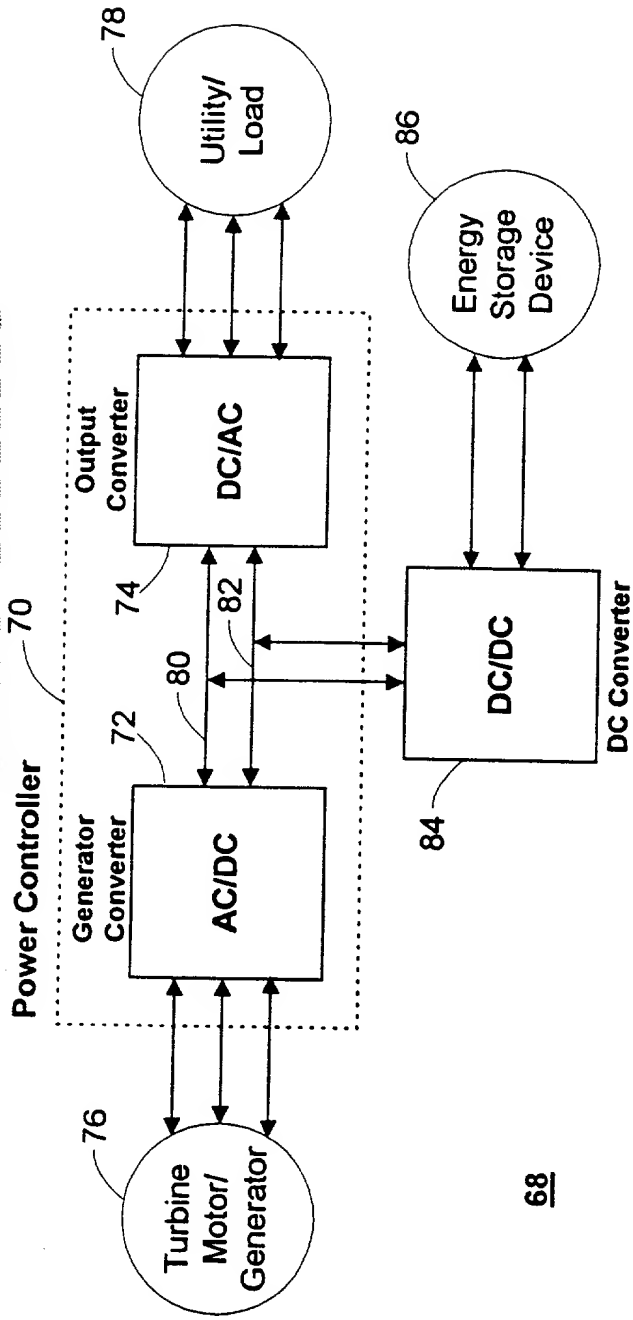


FIG. 4

68

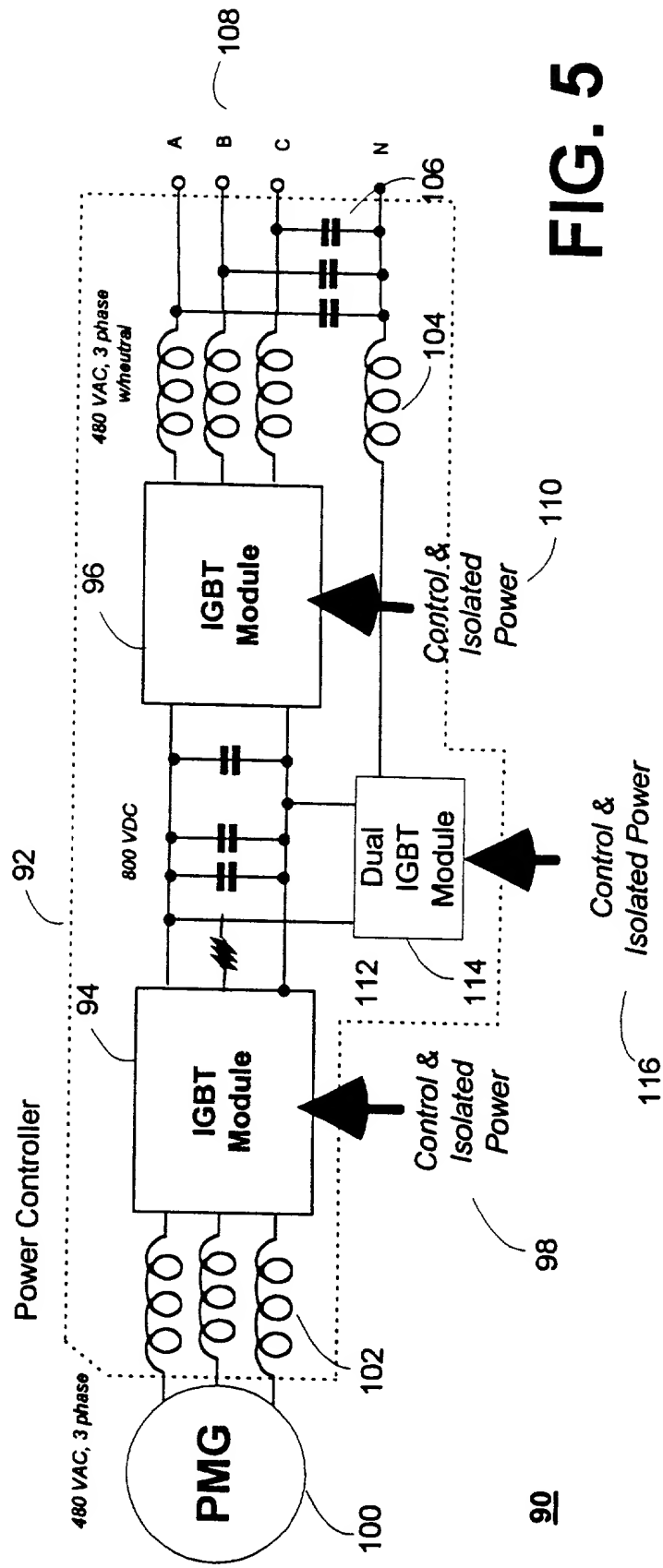


FIG. 5

90

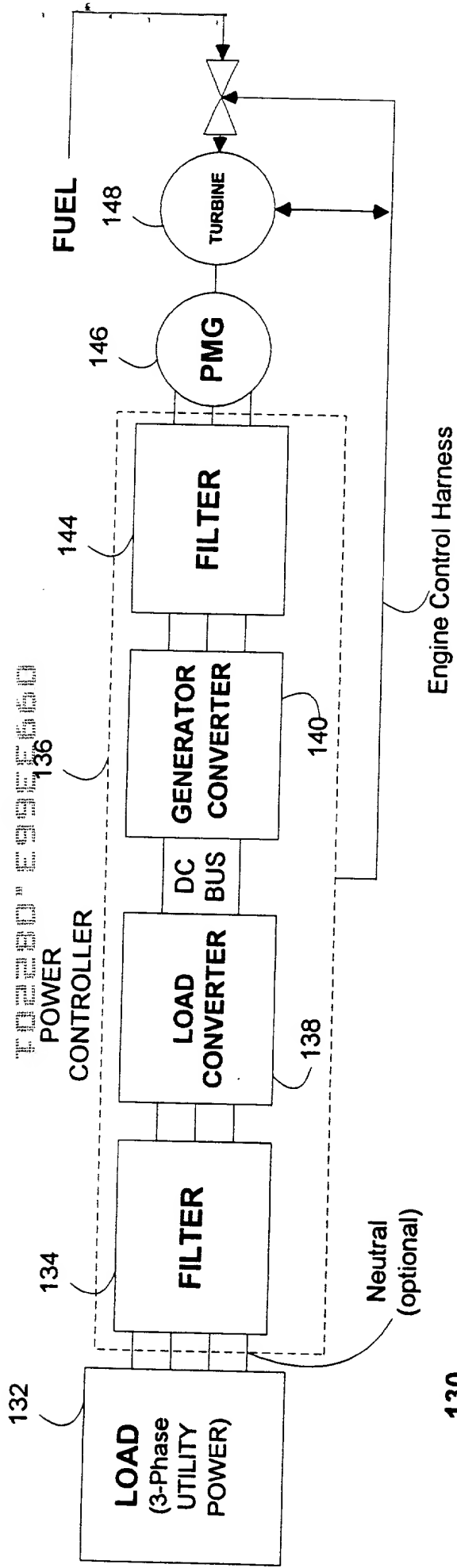


FIG. 6

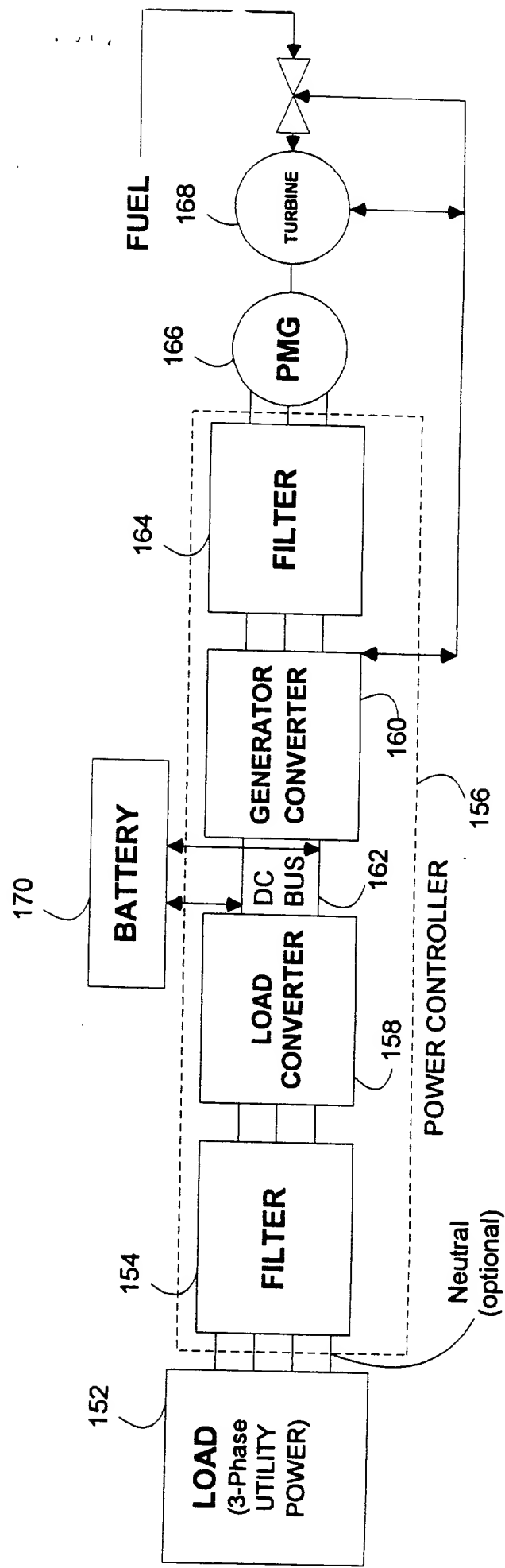
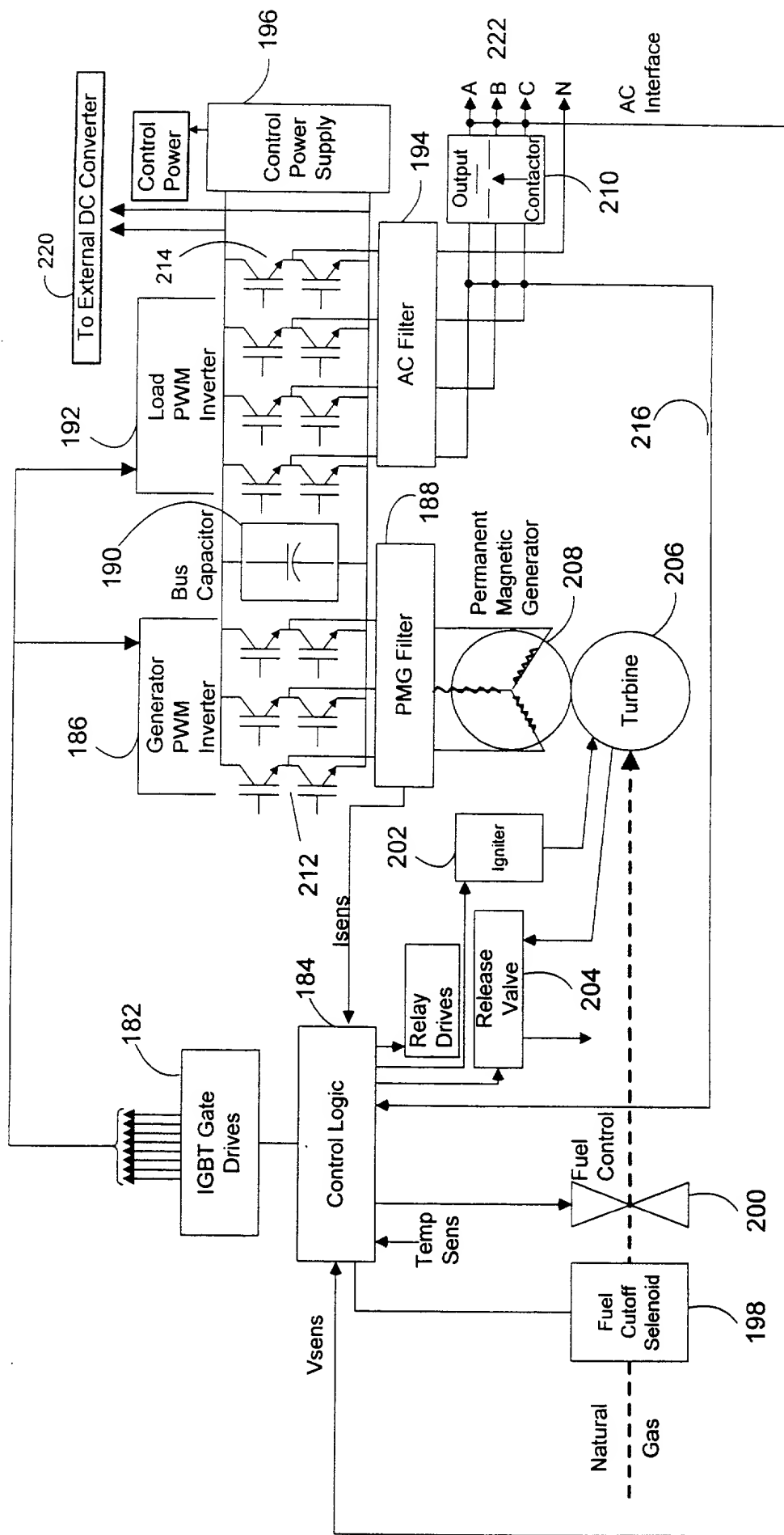


FIG. 7



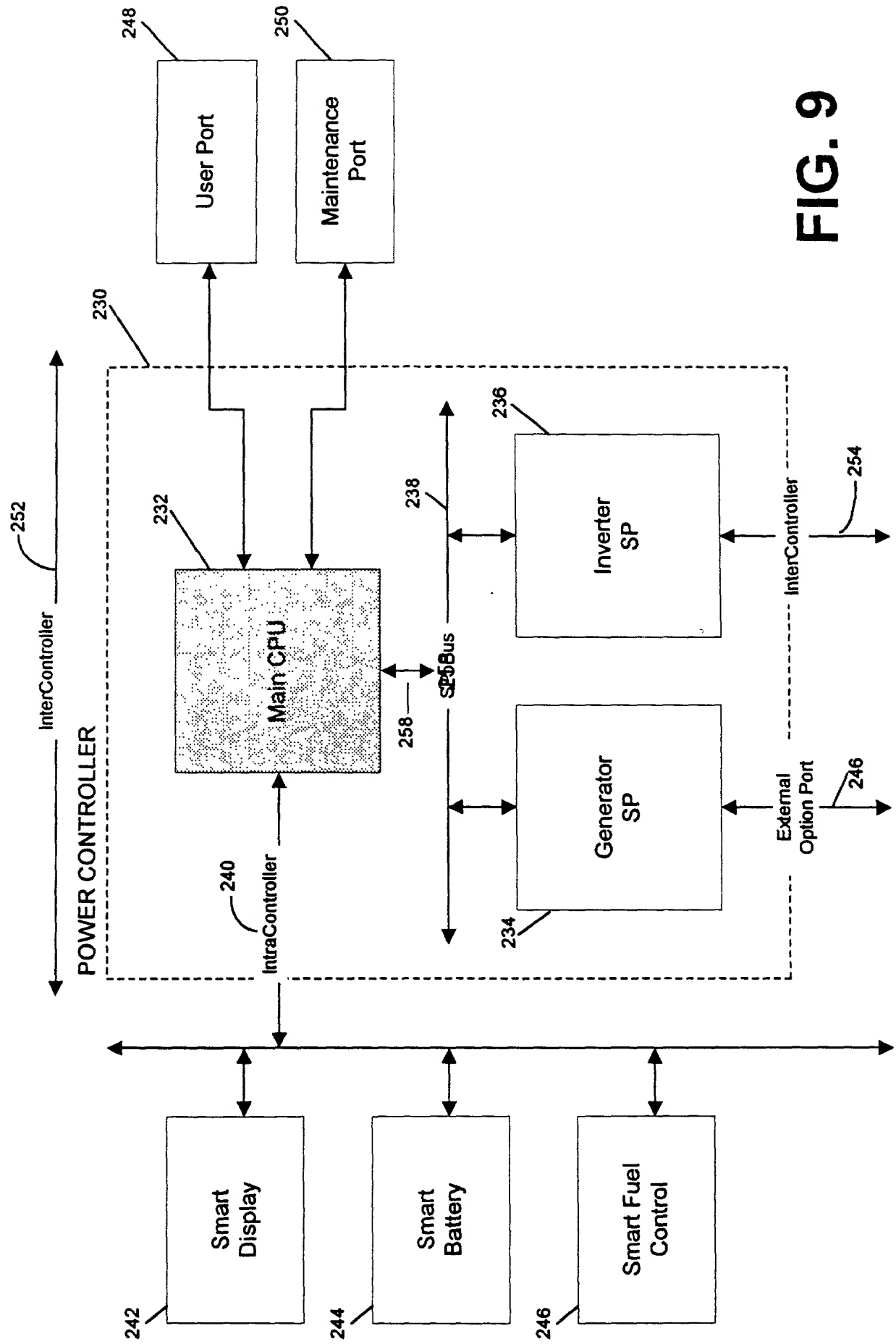
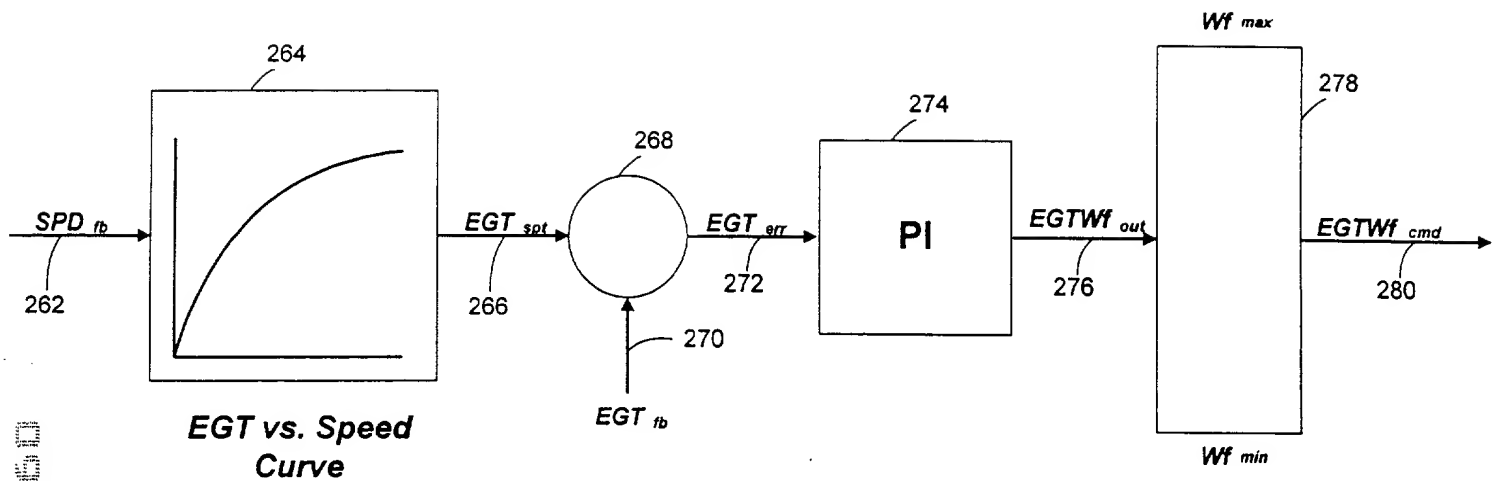
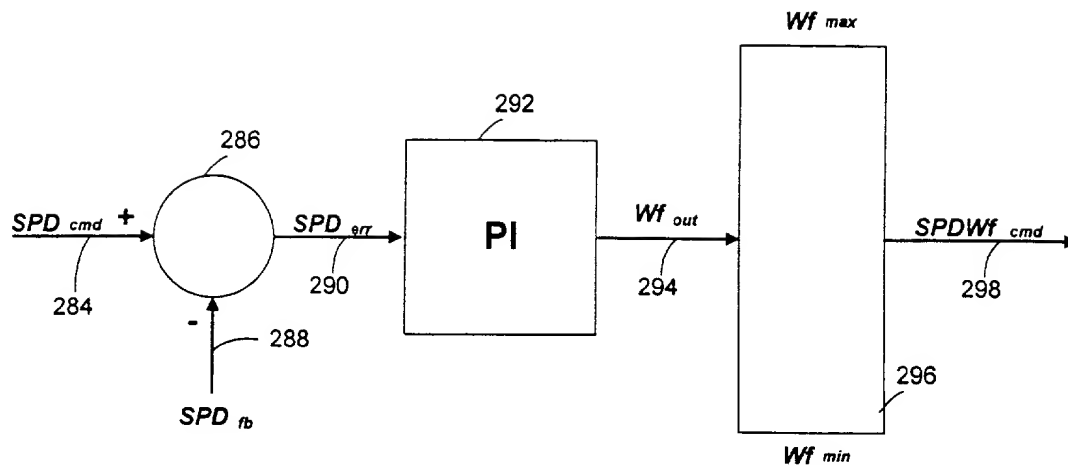


FIG. 9



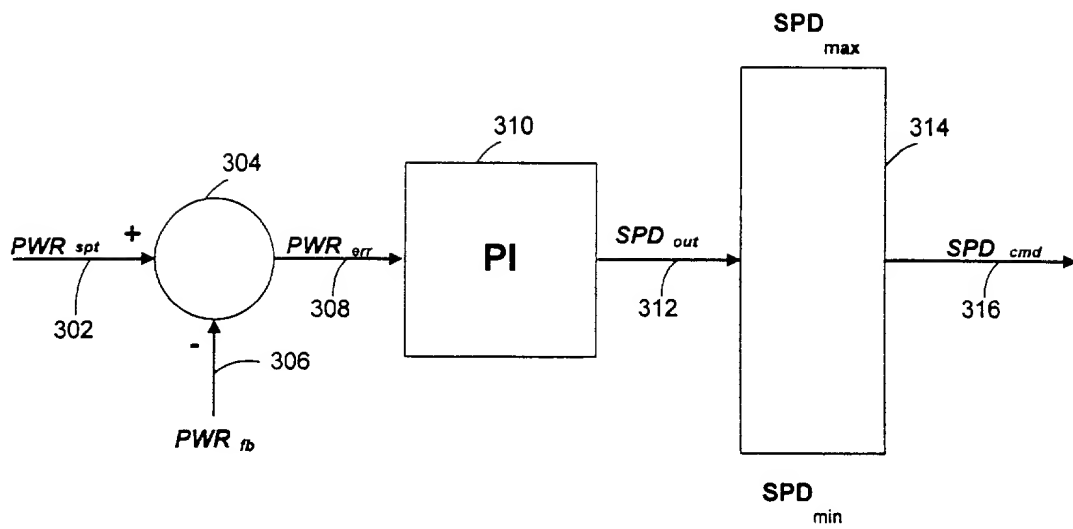
260

FIG. 10



282

FIG. 11



300

FIG. 12

336'

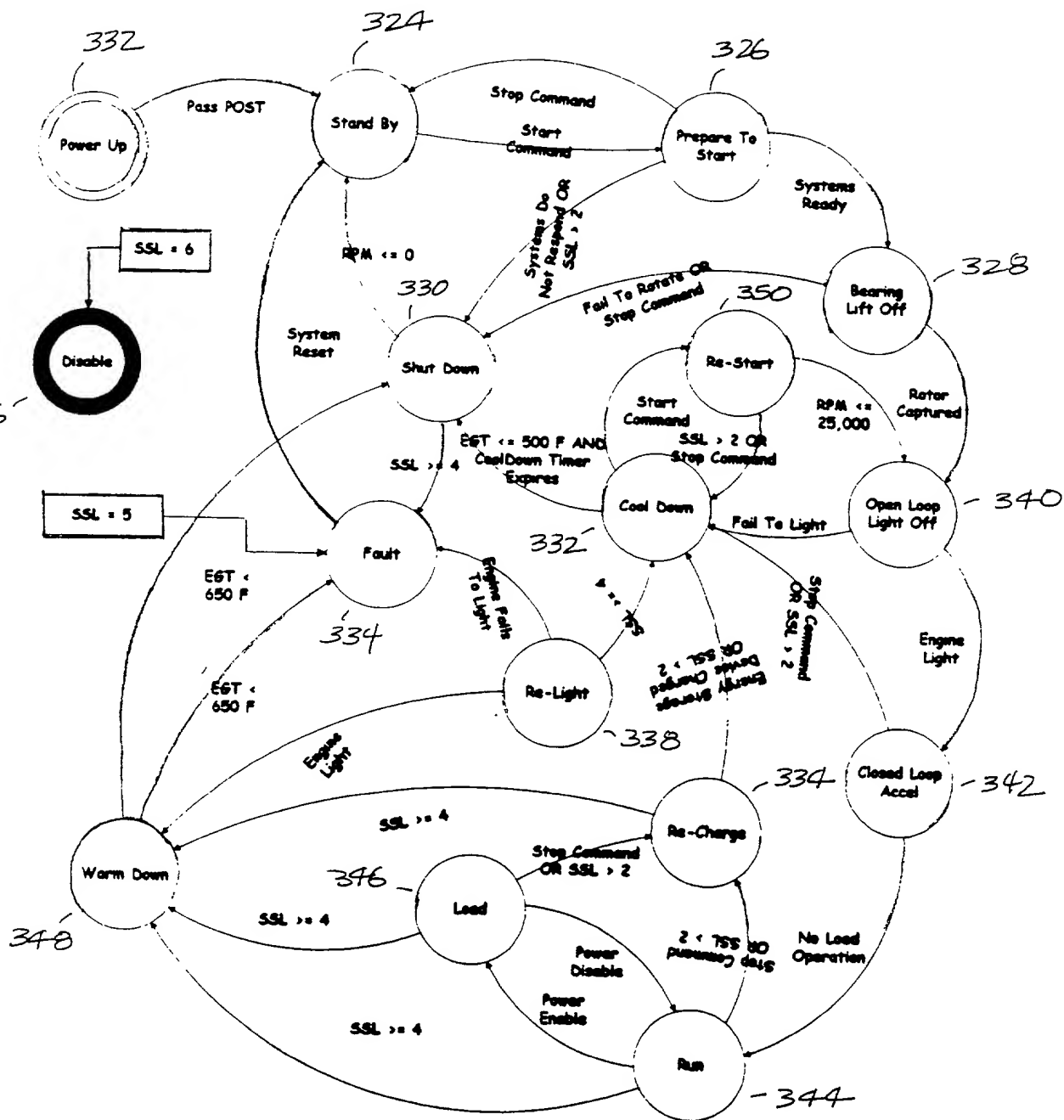
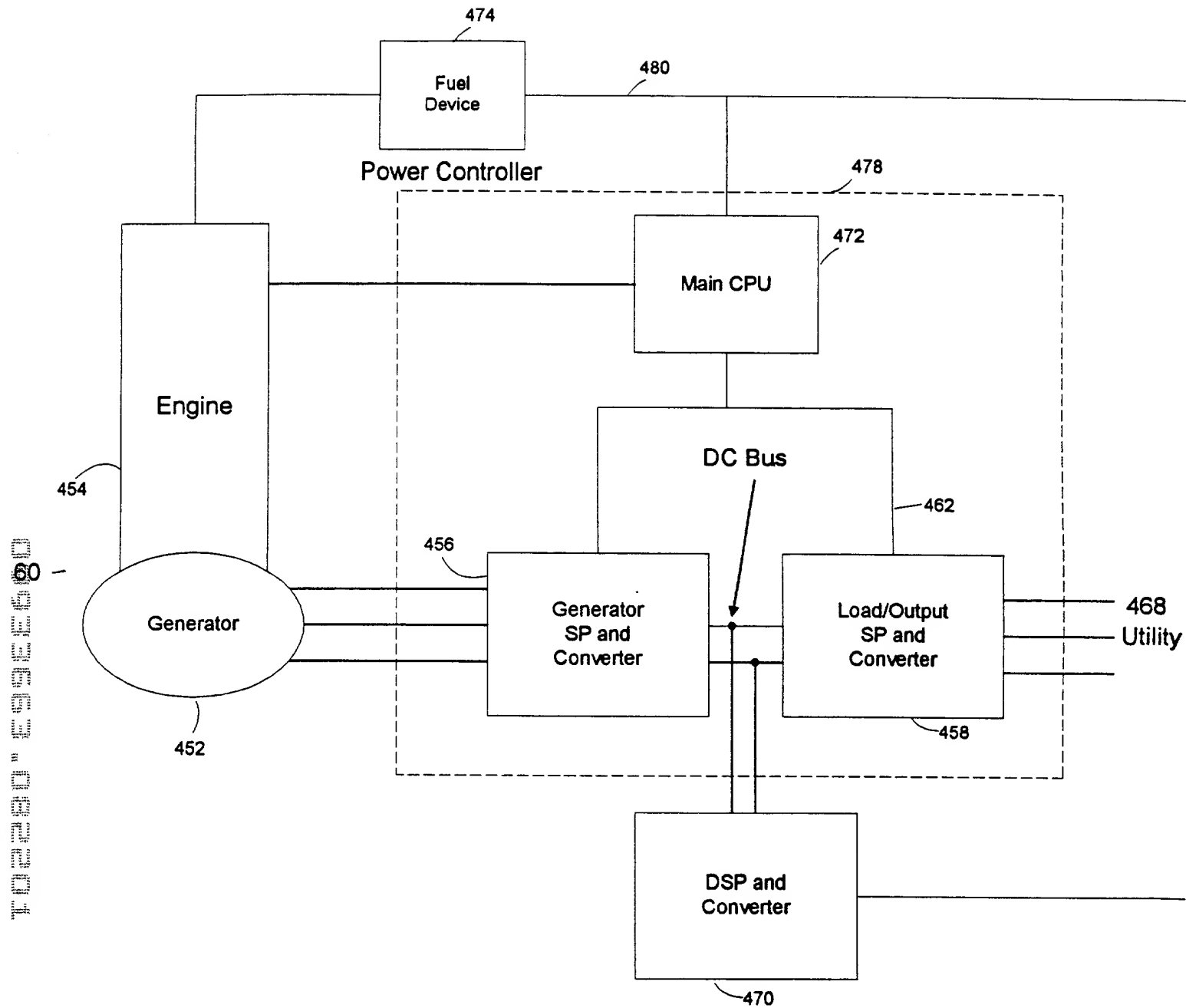


FIG. 13



450

FIG. 14

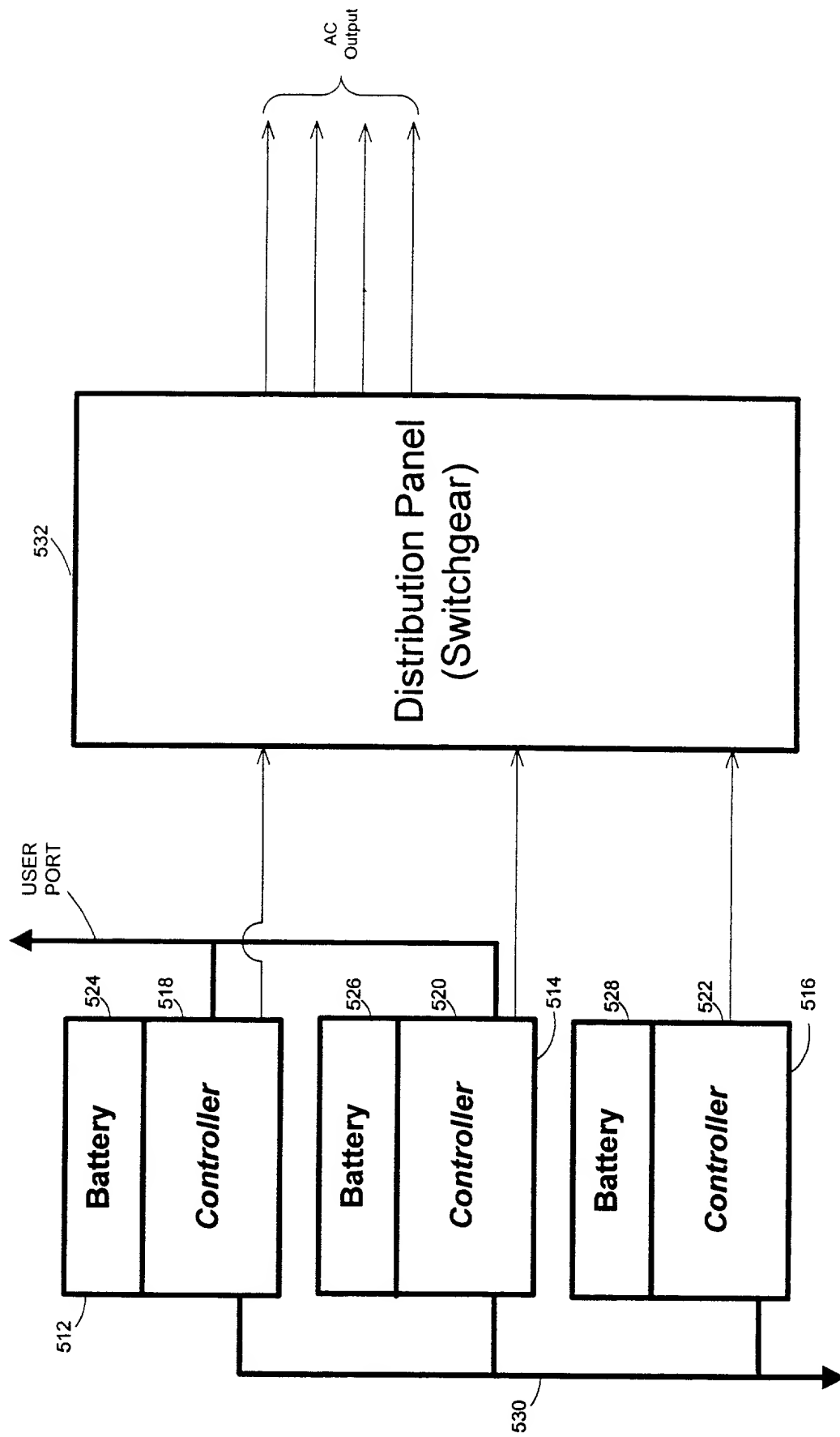


FIG. 15

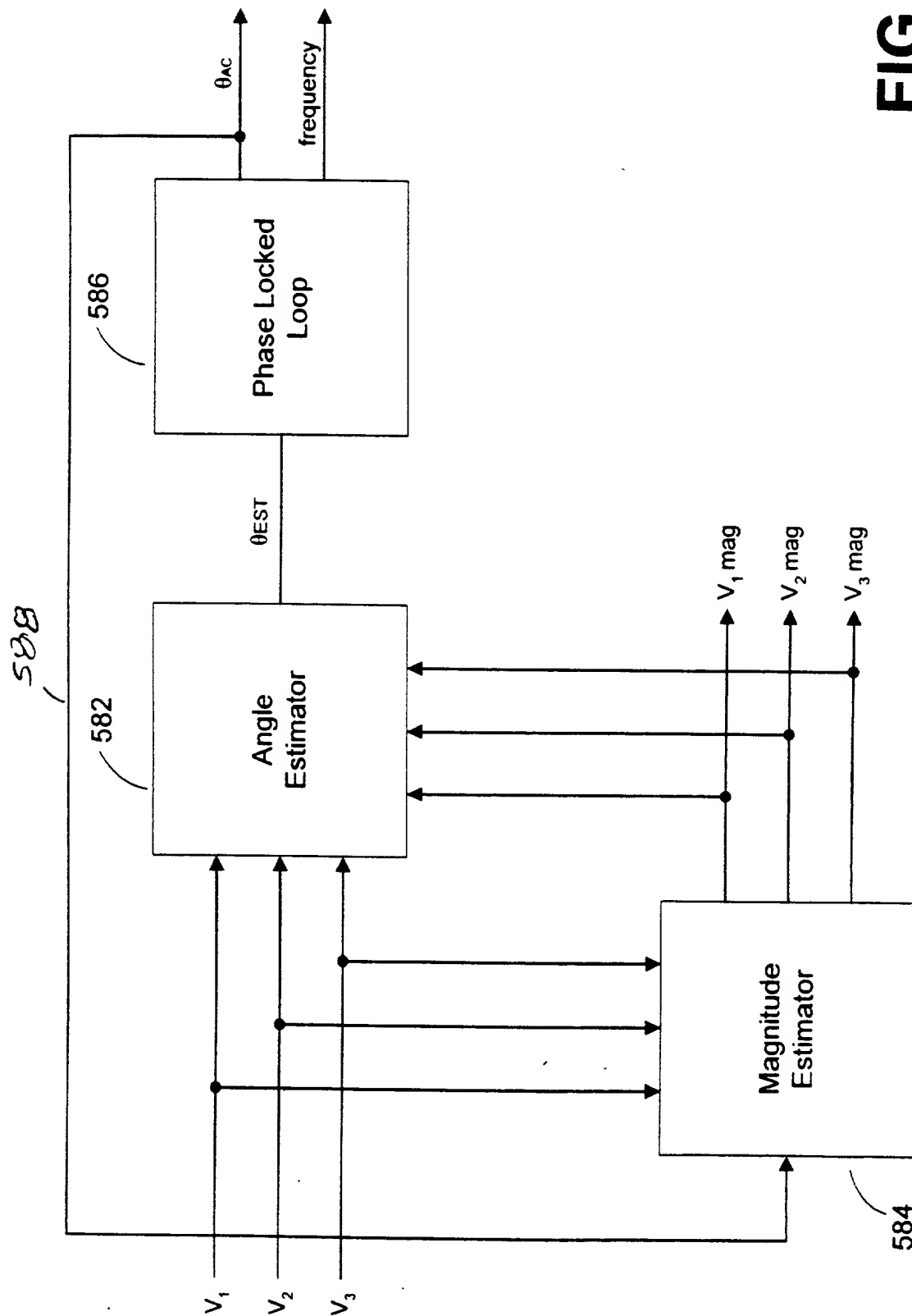


FIG. 16

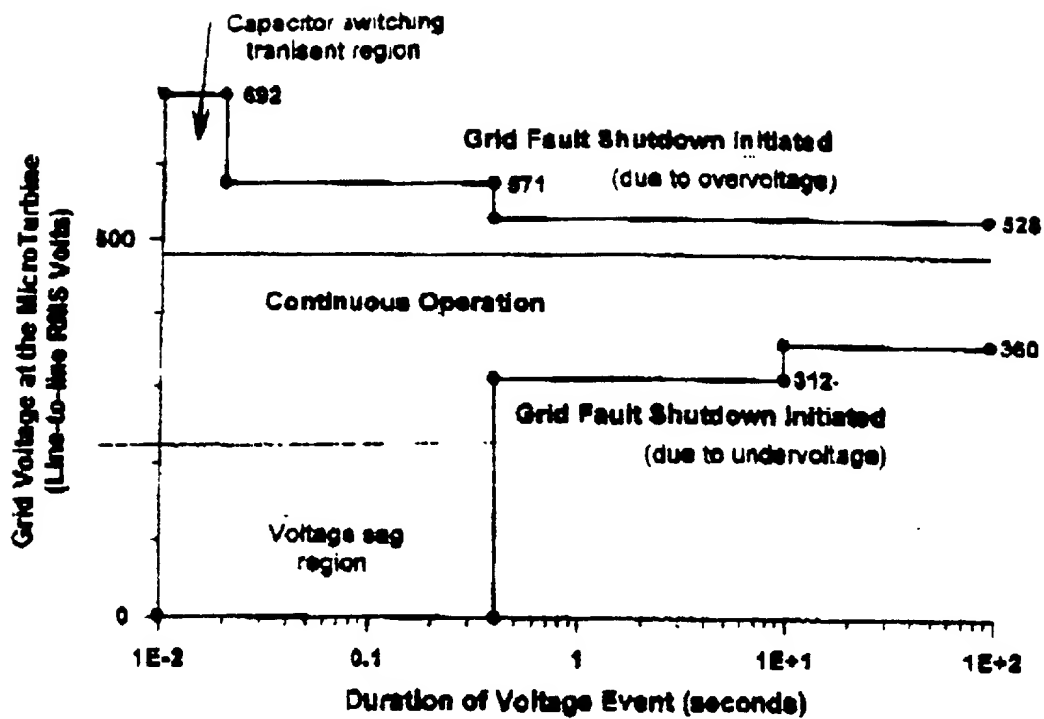
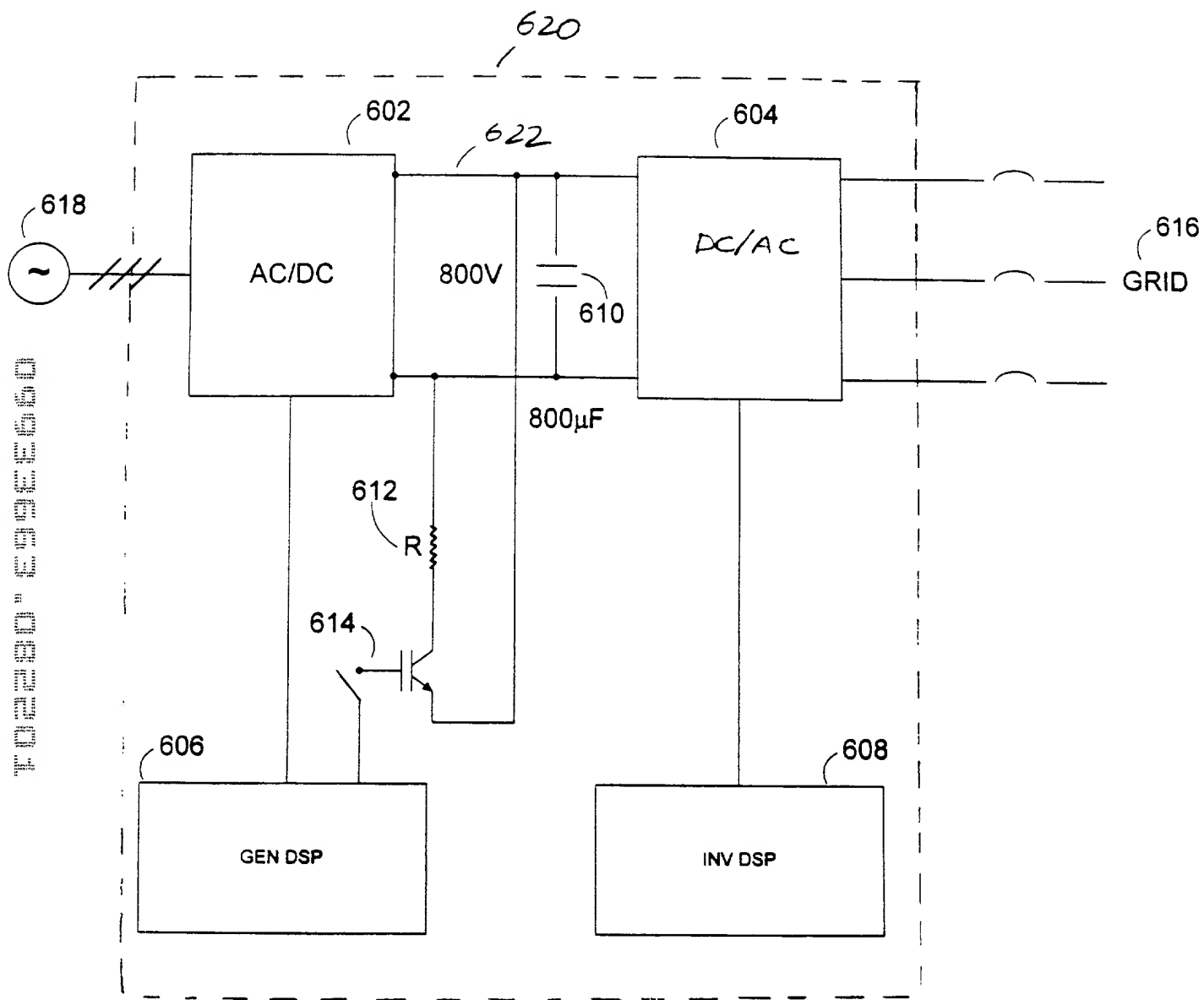


FIG. 17



600

FIG. 18

Appendix B

ANALYSIS OF EMISSION CONTROL BY A CATALYTIC RECUPERATOR AND BY UPSTREAM MONOLITHS

INTRODUCTION

[REDACTED]
[REDACTED] using post turbine catalytic monoliths and catalytically active exhaust-side recuperator surfaces to remove hydrocarbon and carbon monoxide emissions from the Capstone turbogenerators. [REDACTED]
[REDACTED]

[REDACTED] This report represents the detailed analysis, calculations, results, and conclusions. Also attached are the MathSoft Mathcad™ 6+ documents comprising the analyses and an Excel 5.0 spreadsheet of the findings.

TRANSPORT AND KINETIC ANALYSIS OF THE RECUPERATOR AND MONOLITHS

The analysis of the conversion of heptene (C_7H_{14}), methane (CH_4), and carbon monoxide (CO), were completed for several configurations of a recuperator and honeycomb catalytic converters. The method used was a MATHCAD program, and the procedures were similar to the document sent to Capstone [REDACTED] (CAPSTONE.MCD document).

The analyses consist of the following features (see printouts for CPSTONE5.MCD and CPSTONE6.MCD):

Gas Properties

- The properties of the gases used in the combustion mixture are described on pages 1-8.
- The gas compositions both for complete combustion air with fuel equivalence ratio 0.1 in moist (2 vol% water vapor) air, as specified in the problem statement, and also for an adiabatic temperature rise from 1000° to 1511_F using heptene are defined on page 2. The difference in properties between these two compositions is insignificant.
- Essential transport properties, such as the diffusivities of the added gases are determined on pages 3-4.
- Mixture properties such as viscosity, thermal conductivity, heat capacity, and various dimensionless transport numbers such as the Prandtl and Schmidt numbers are defined and calculated on pages 5-8.

Recuperator and Converter Dimensions and Operating Conditions

- The dimensions of the honeycomb sizes from 100 to 800 cells/in.² are defined on page 9 along with the size and dimensions of the recuperator and the upstream monolith converters.
- The five operating combustion conditions representing the different power level cases for the turbogenerator are specified on pages 9-10.
- The pressure drop for the 600 or 800 cells/in.² recuperator is determined on page 11, and the analysis of heat transfer within the recuperator is described on page 12.

Recuperator Performance

- Mass transfer rates to the wall of the recuperator (assuming very fast conversion kinetics at the wall) are described on pages 13-14 for all three added components (C₇H₁₄, CH₄, and CO). These calculations used average temperatures to determine an integrated formula for fuel conversion.
- An alternative form of conversion was developed by looking at local Nusselt number (modified for the square channel configuration). This analysis is described on pages 15 and 16. The two methods show good agreement for C₇H₁₄ conversion.
- Catalytic properties and functions are defined on pages 17-18, and the specific rate expression for oxidation of dilute CH₄ by supported palladium oxide (PdO) is described on page 19.
- Slow (in CPSTONE5.MCD and related to the rate of CH₄ oxidation) and moderate (in CPSTONE6.MCD and related to the rate of C₃H₆ oxidation) rate constants for C₇H₁₄ oxidation are described on p. 19.
- The performance of the recuperator for conversion with temperature-dependent mass transfer properties and specific catalytic rates for C₇H₁₄ and CH₄ are described on pages 20-21.

Performance of Upstream Monoliths

- The operating conditions for 200, 400, and 600 cells/in.² honeycombs is described on pages 22-25.
- The pressure drop for three honeycombs (200, 400, and 600 cells/in.²) is described on pages 22-23, and matched to the maximum specified conditions. From of these calculations, two honeycomb converter configurations, 400 cells/in.² by 4 in. length and 600 cells/in.² by 3.5 in. length, were chosen for mass transfer calculations.
- The effluent concentrations of added components are calculated for the constant temperature monoliths (400 cells/in.² in CPSTONE5.MCD and 600 cells/in.² in CPSTONE6.MCD) for the five operating conditions (cases) on pages 24-25, assuming very fast catalytic rates.
- Finally, on pages 25-27, the conversion of C₇H₁₄ and CH₄ using finite catalytic rates are described for the honeycomb converters (400 cells/in.² in CPSTONE5.MCD and 600 cells/in.² in CPSTONE6.MCD).

RESULTS OF THE ANALYSIS

The principal results of the analysis of post turbine fuel component conversion are shown in the attached spreadsheet tables (CAPSTN5.XLS) and Mathcad documents (CPSTONE5.MCD and CPSTONE6.MCD). The main results of the analyses are summarized as follows:

Catalytic Recuperator

- The $\Delta P/P$ calculations seem to very closely fit your measured values. [REDACTED] We chose as the best calculation of pressure drop an 800 cells/in² x 7-in. with 10% additional added length to describe the chevron geometry of the recuperator foils.
- The estimated averaged wall temperatures, or skin temperatures, within the recuperator seemed a little low (< 50°F) based on [REDACTED] discussions of recuperator thermal efficiency. As a consequence, the cell size was increased to 600 cells/in² keeping the length the same (7 in. x 1.1) for a conservative calculation of mass transfer rates.
- For the mass transfer limited cases (assuming fast kinetics), virtually complete conversion CH₄ and CO is predicted (see Table of Results 1). Except at the highest power level, conversion of CH₄ and CO was essentially complete within the first inch or two of entry into the recuperator.
- For the transport-limited cases with C₇H₁₄, maximum conversions are low only for Case 5 (full power). Even in this case, 50 ppm would be converted to < 1 ppm (0.2 ppm) while concentrations entering the recuperator above 250 ppm would exit at levels above 1 ppm (500 ppm \Rightarrow 2.1 ppm). The situation improves for the other cases (e.g., Case 4 gives 500 ppm \Rightarrow 0.02 ppms while 5000 ppm \Rightarrow 0.17 ppm).
- Conversions would be much higher for transport limited conversion in a the 800 cells/in.² recuperator, as calculations with this cell size were found reproduce the observed pressure drop. In this case, the logarithm of the inlet concentration divided by the outlet concentration for all added components would be ~35 % greater with the smaller cell size.
- The step-wise calculation which includes the temperature on flow velocity and transport properties showed reasonably good agreement with the integrated calculation using average properties. This method gave lower overall conversion than the averaged property formulas, but the results were close. Perhaps the higher property values at the inlet, particularly the greater velocity, more than offset the lower transport values at the outlet side.
- CH₄ conversion is catalytically rate limited under all conditions (see Table of Results 1). Conversions were calculated to be very low, with a maximum conversion of ~66% under Case 1 and ~32% conversion under Case 5. These conversions would increase somewhat, perhaps by a factor of 2, with the use of a thicker coating (e.g., 25 μ m vs. 10 μ m).
- CO conversion is likely to exceed 99% in all operating conditions for the recuperator. This is because the kinetics of CO conversion are probably much faster than CH₄ and may well be close to the transport-limited case, at least through the (hotter) first several inches of the recuperator where most of the CO would be consumed.

- The catalytic recuperator, C_7H_{14} rate determines its conversion in the recuperator conditions (see Table of Results 1). For the slower rates (derived from the rates for CH_4 oxidation) using the 600 cells/in.² value for recuperator cell size, we find a range from 99.4% conversion under Case 1 to about 85.6% under Case 5. If twice the rate of combustion of propane is extrapolated to the higher temperatures of the recuperator, much higher C_7H_{14} conversions result, 99.98% under Case 1, and 96.4% under Case 5.

Catalytic Monoliths

- The pressure drop reaches maximum specifications for the 400 cells/in.² honeycomb at 4-in. length. Maximum pressure drop would be reached in a shorter (~3.5 in. length) 600 cells/in.² monolith. Both configurations were chosen for analysis (CPSTONE5.MCD for 400 cells/in.² and CPSTONE6.MCD for 600 cells/in.²).
- Transport-limited conversion shows excellent performance for methane and CO in all cases, including the full-power case, for both honeycomb configurations (see Table of Results 2).
- As for the recuperator, methane conversion is again reaction rate limited (see Table of Results 3), with conversions range from 93.8% under Case 1 with the 600 cells/in.² monolith to only 31% conversion under Case 5 for the 400 cells/in.² monolith.
- C_7H_{14} conversions under transport-limited conditions depends on the specific configuration (see Table of Results 2). For the 600 cells/in.² monolith conversions are very high for Case 1, but fall to about 92% for Case 5. With the 400 cells/in.² configuration, these fast kinetic transport-limited conversions fall to 87% conversion under Case 5.
- The reaction rate of C_7H_{14} strongly affects its conversion in either honeycomb monolith (see Table of Results 3). For the extrapolated propane kinetics at 600 cells/in.², 98% conversion is expected under Case 5, whereas the 400 cells/in.² using the more conservative extrapolation using PdO methane kinetics, 86% conversion is expected under Case 5.

Effect of Washcoat Thermal Conductivity in a Recuperator

- The application of a thin washcoat of porous alumina gives a very slight *increase* in the overall heat transfer coefficient (CPSNALT2.MCD). The thermal conductivity of the washcoat, while significantly less than that of stainless 321, is greater than that of the gas phase boundary. Because the washcoat displaces the gas phase (creating a narrower channel) it causes a slight increase in overall heat transfer coefficient.

OVERALL CONCLUSIONS AND RECOMMENDATIONS

The conclusions and recommendations drawn from the results of the analysis is listed below:

- 1) The actual C_7H_{14} outlet concentration from the turbine are needed to assess the effluent emissions in the high-power case (Case 5) for either control strategy. Provided that fast catalytic rates can be provided in washcoats on either the recuperator or upstream monoliths, maximum conversions for C_7H_{14} under full power range from 99.6% (for an effective cell size of 600 cells/in²) to > 99.9% (if the effective cell size is 800 cells/in²).
- 2) The two methods (averaged properties and integrated formulas vs. local temperature dependent properties and finite difference integration) show good agreement for recuperator performance with infinitely fast catalytic reactions at the wall.
- 3) Clearly, it will be necessary to apply and measure specific catalytic rates for C_7H_{14} or gasoline to be sure that these estimated conversions could be achieved under actual operating conditions for either the catalytic recuperator or the upstream honeycomb monoliths.
- 4) Thin wash coats (< 20 μm) should have minimal effect on the transport of heat through the recuperator given the much greater resistance of the gas phase boundary layers.
- 5) For the current operating conditions, use of a standard 400 cells/in² x 4-in length catalytic monolith upstream of the recuperator is recommended.
- 6) If the recuperator temperature can be raised (~ 200°F) high conversions of CO, C_7H_{14} , and even CH_4 can be expected under all flow conditions. In this case it is possible that only the first 3 to 4 inches of the recuperator be wash coated with catalyst because the downstream wall temperatures are too cool to be effective.

Recupercator - Transport only (assumes fast reaction kinetics) at 600 cells/in2												
Inlet (added component) conc(ppm)	Case-1			Case-2			Case-3			Case-4		
	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO
5000	2.011E-25	3.554E-05	5.555E-23	3.704E-19	0.002197	3.002E-17	1.373E-15	0.022964	5.542E-14	1.470E-12	0.1687	3.276E-11
2000	8.046E-26	1.422E-05	2.222E-23	1.481E-19	8.787E-04	1.201E-17	5.492E-16	0.009186	2.217E-14	5.880E-13	0.0574683	1.310E-11
1000	4.023E-26	7.108E-06	1.111E-23	7.407E-20	4.393E-04	6.003E-18	2.746E-16	0.004593	1.108E-14	2.940E-13	0.0337341	6.552E-12
500	2.011E-26	3.554E-06	5.555E-24	3.704E-20	2.197E-04	3.002E-18	1.373E-16	0.002296	5.542E-15	1.470E-13	0.0168671	3.276E-12
200	8.046E-27	1.422E-06	2.222E-24	1.481E-20	8.787E-05	1.201E-18	5.492E-17	9.186E-04	2.217E-15	5.880E-14	0.0067468	1.310E-12
100	4.023E-27	7.108E-07	1.111E-24	7.407E-21	4.393E-05	6.003E-19	2.746E-17	4.593E-04	1.108E-15	2.940E-14	0.0033734	6.552E-13
50	2.011E-27	3.554E-07	5.555E-25	3.704E-21	2.197E-05	3.002E-19	1.373E-17	2.296E-04	5.542E-16	1.470E-14	0.0018687	3.276E-13
20	8.046E-28	1.422E-07	2.222E-25	1.481E-21	8.787E-06	1.201E-19	5.492E-18	9.186E-05	2.217E-16	5.880E-15	6.747E-04	1.310E-13
10	4.023E-28	7.108E-08	1.111E-25	7.407E-22	4.393E-06	6.003E-20	2.746E-18	4.593E-05	1.108E-16	2.940E-15	3.373E-04	6.552E-14
5	2.011E-28	3.554E-08	5.555E-26	3.704E-22	2.197E-06	3.002E-20	1.373E-18	2.296E-05	5.542E-17	1.470E-15	1.887E-04	3.276E-14
2	8.046E-29	1.422E-08	2.222E-26	1.481E-22	8.787E-07	1.201E-20	5.492E-19	9.186E-06	2.217E-17	5.880E-16	6.747E-05	1.310E-14
1	4.023E-29	7.108E-09	1.111E-26	7.407E-23	4.393E-07	6.003E-21	2.746E-19	4.593E-06	1.108E-17	2.940E-16	3.373E-05	6.552E-15

Recupercator - C7H14 without reaction with T-dependence (step) and CH4 and C7H14 with finite catalytic reaction rates at the wall (C7H14 rate = 10 x CH4 rate - slow kinetics)

Inlet conc(ppm)	Case-1			Case-2			Case-3			Case-4			Case-5		
	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react
5000	3.201E-04	1.675E-01	3.158E-01	0.012075	2.081E-01	82.9500	0.094050	2.310E-01	133.15	0.5350	2.543E-01	217.85	34.8470	3420.30	707.30
2000	1.280E-04	673.00	12.6340	0.004830	826.00	331.8000	0.037620	324.00	55.8500	0.2140	1018.00	87.1400	13.9350	1363.00	263.00
1000	6.402E-05	336.00	6.3170	0.002415	413.00	16.5900	0.018810	162.00	27.8300	0.1070	509.00	43.5700	6.9690	684.00	141.50
500	3.201E-05	167.50	3.1580	0.001208	208.00	8.2950	0.009405	81.00	13.9150	0.053500	254.00	21.7850	3.4840	342.00	70.7500
200	1.280E-05	67.0000	1.2634	0.000483	82.6000	3.3180	0.003762	32.4000	5.5860	0.021400	101.80	8.7140	1.3936	136.00	26.3000
100	6.402E-06	33.5000	0.6317	0.000242	41.3000	1.6590	0.001881	16.2000	2.7830	0.010700	50.9000	4.3570	0.6968	68.4000	14.1500
50	3.201E-06	16.7500	0.3158	0.000121	20.8000	0.8295	0.000940	8.2000	1.3915	0.005350	25.4500	2.1785	0.3484	34.2000	7.0750
20	1.280E-06	6.7000	0.1263	0.000048	8.2600	0.3318	0.000483	3.2600	0.5586	0.002140	10.1800	0.8714	0.1394	13.6800	2.6300
10	6.402E-07	3.3500	0.063170	2.415E-05	4.1300	0.1659	1.881E-04	1.6200	0.2783	0.001070	5.0900	0.4357	0.069690	6.8400	1.4150
5	3.201E-07	1.6750	0.031585	1.208E-05	2.0650	0.082950	9.405E-05	0.8100	0.1392	5.350E-04	2.5450	0.2179	0.034840	3.4200	0.7075
2	1.280E-07	0.6700	0.012634	4.830E-06	0.8260	0.033180	3.762E-05	0.3240	0.055660	2.140E-04	1.0180	0.0871	0.013936	1.3680	0.2630
1	6.402E-08	0.3350	0.006317	2.415E-06	0.4130	0.016590	1.881E-05	0.1620	0.027890	1.070E-04	0.5090	0.0436	0.006968	0.6840	0.1415

Case# : 1 2 3 4 5
lnf(youthyln)

CH4:	-65.383	-50.957	-42.739	-35.763	-18.994
C7H14	-18.762	-14.638	-12.291	-10.297	-5.49
CO	-59.762	-46.562	-39.041	-32.659	-17.344
C7H14step	-16.56407	-12.933811	-10.88112	-9.142682	-4.966427
CH4react	-1.0936247	-0.8843077	-0.77219	-0.675307	-0.379797
C7H14react	-5.0845108	-4.0989552	-3.581641	-3.133386	-1.955456

BL transport only with averaged integrated values
 BL transport only with averaged integrated values
 BL transport only with averaged integrated values
 BL transport only with T-dependent properties and step-wise integration
 BL transport-restricted catalytic rates with T-dependent properties and step-wise integration
 BL transport-restricted catalytic rates with T-dependent properties and step-wise integration

Table of Results 2

Inlet (added component)		Transport only (assumes fast reaction kinetics) for a 600 cells/in ² x 3.5-in length square honeycomb monolith										Transport only (assumes fast reaction kinetics) for a 400 cells/in ² x 4-in length square honeycomb monolith										Transport only (assumes fast reaction kinetics) for a 200 cells/in ² x 5-in length square honeycomb monolith																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
		Case-1		Case-2		Case-3		Case-4		Case-5		Case-6		Case-7		Case-8		Case-9		Case-10		Case-11		Case-12		Case-13		Case-14		Case-15		Case-16		Case-17		Case-18		Case-19		Case-20		Case-21		Case-22		Case-23		Case-24		Case-25		Case-26		Case-27		Case-28		Case-29		Case-30		Case-31		Case-32		Case-33		Case-34		Case-35		Case-36		Case-37		Case-38		Case-39		Case-40		Case-41		Case-42		Case-43		Case-44		Case-45		Case-46		Case-47		Case-48		Case-49		Case-50		Case-51		Case-52		Case-53		Case-54		Case-55		Case-56		Case-57		Case-58		Case-59		Case-60		Case-61		Case-62		Case-63		Case-64		Case-65		Case-66		Case-67		Case-68		Case-69		Case-70		Case-71		Case-72		Case-73		Case-74		Case-75		Case-76		Case-77		Case-78		Case-79		Case-80		Case-81		Case-82		Case-83		Case-84		Case-85		Case-86		Case-87		Case-88		Case-89		Case-90		Case-91		Case-92		Case-93		Case-94		Case-95		Case-96		Case-97		Case-98		Case-99		Case-100		Case-101		Case-102		Case-103		Case-104		Case-105		Case-106		Case-107		Case-108		Case-109		Case-110		Case-111		Case-112		Case-113		Case-114		Case-115		Case-116		Case-117		Case-118		Case-119		Case-120		Case-121		Case-122		Case-123		Case-124		Case-125		Case-126		Case-127		Case-128		Case-129		Case-130		Case-131		Case-132		Case-133		Case-134		Case-135		Case-136		Case-137		Case-138		Case-139		Case-140		Case-141		Case-142		Case-143		Case-144		Case-145		Case-146		Case-147		Case-148		Case-149		Case-150		Case-151		Case-152		Case-153		Case-154		Case-155		Case-156		Case-157		Case-158		Case-159		Case-160		Case-161		Case-162		Case-163		Case-164		Case-165		Case-166		Case-167		Case-168		Case-169		Case-170		Case-171		Case-172		Case-173		Case-174		Case-175		Case-176		Case-177		Case-178		Case-179		Case-180		Case-181		Case-182		Case-183		Case-184		Case-185		Case-186		Case-187		Case-188		Case-189		Case-190		Case-191		Case-192		Case-193		Case-194		Case-195		Case-196		Case-197		Case-198		Case-199		Case-200		Case-201		Case-202		Case-203		Case-204		Case-205		Case-206		Case-207		Case-208		Case-209		Case-210		Case-211		Case-212		Case-213		Case-214		Case-215		Case-216		Case-217		Case-218		Case-219		Case-220		Case-221		Case-222		Case-223		Case-224		Case-225		Case-226		Case-227		Case-228		Case-229		Case-230		Case-231		Case-232		Case-233		Case-234		Case-235		Case-236		Case-237		Case-238		Case-239		Case-240		Case-241		Case-242		Case-243		Case-244		Case-245		Case-246		Case-247		Case-248		Case-249		Case-250		Case-251		Case-252		Case-253		Case-254		Case-255		Case-256		Case-257		Case-258		Case-259		Case-260		Case-261		Case-262		Case-263		Case-264		Case-265		Case-266		Case-267		Case-268		Case-269		Case-270		Case-271		Case-272		Case-273		Case-274		Case-275		Case-276		Case-277		Case-278		Case-279		Case-280		Case-281		Case-282		Case-283		Case-284		Case-285		Case-286		Case-287		Case-288		Case-289		Case-290		Case-291		Case-292		Case-293		Case-294		Case-295		Case-296		Case-297		Case-298		Case-299		Case-300		Case-301		Case-302		Case-303		Case-304		Case-305		Case-306		Case-307		Case-308		Case-309		Case-310		Case-311		Case-312		Case-313		Case-314		Case-315		Case-316		Case-317		Case-318		Case-319		Case-320		Case-321		Case-322		Case-323		Case-324		Case-325		Case-326		Case-327		Case-328		Case-329		Case-330		Case-331		Case-332		Case-333		Case-334		Case-335		Case-336		Case-337		Case-338		Case-339		Case-340		Case-341		Case-342		Case-343		Case-344		Case-345		Case-346		Case-347		Case-348		Case-349		Case-350		Case-351		Case-352		Case-353		Case-354		Case-355		Case-356		Case-357		Case-358		Case-359		Case-360		Case-361		Case-362		Case-363		Case-364		Case-365		Case-366		Case-367		Case-368		Case-369		Case-370		Case-371		Case-372		Case-373		Case-374		Case-375		Case-376		Case-377		Case-378		Case-379		Case-380		Case-381		Case-382		Case-383		Case-384		Case-385		Case-386		Case-387		Case-388		Case-389		Case-390		Case-391		Case-392		Case-393		Case-394		Case-395		Case-396		Case-397		Case-398		Case-399		Case-400		Case-401		Case-402		Case-403		Case-404		Case-405		Case-406		Case-407		Case-408		Case-409		Case-410		Case-411		Case-412		Case-413		Case-414		Case-415		Case-416		Case-417		Case-418		Case-419		Case-420		Case-421		Case-422		Case-423		Case-424		Case-425		Case-426		Case-427		Case-428		Case-429		Case-430		Case-431		Case-432		Case-433		Case-434		Case-435		Case-436		Case-437		Case-438		Case-439		Case-440		Case-441		Case-442		Case-443		Case-444		Case-445		Case-446		Case-447		Case-448		Case-449		Case-450		Case-451		Case-452		Case-453		Case-454		Case-455		Case-456		Case-457		Case-458		Case-459		Case-460		Case-461		Case-462		Case-463		Case-464		Case-465		Case-466		Case-467		Case-468		Case-469		Case-470		Case-471		Case-472		Case-473		Case-474		Case-475		Case-476		Case-477		Case-478		Case-479		Case-480		Case-481		Case-482		Case-483		Case-484		Case-485		Case-486		Case-487		Case-488		Case-489		Case-490		Case-491		Case-492		Case-493		Case-494		Case-495		Case-496		Case-497		Case-498		Case-499		Case-500		Case-501		Case-502		Case-503		Case-504		Case-505		Case-506		Case-507		Case-508		Case-509		Case-510		Case-511		Case-512		Case-513		Case-514		Case-515		Case-516		Case-517		Case-518		Case-519		Case-520		Case-521		Case-522		Case-523		Case-524		Case-525		Case-526		Case-527		Case-528		Case-529		Case-530		Case-531		Case-532		Case-533		Case-534		Case-535		Case-536		Case-537		Case-538		Case-539		Case-540		Case-541		Case-542		Case-543		Case-544		Case-545		Case-546		Case-547		Case-548		Case-549		Case-550		Case-551		Case-552		Case-553		Case-554		Case-555		Case-556		Case-557		Case-558		Case-559		Case-560		Case-561		Case-562		Case-563		Case-564		Case-565		Case-566		Case-567		Case-568		Case-569		Case-570		Case-571		Case-572		Case-573		Case-574		Case-575		Case-576		Case-577		Case-578		Case-579		Case-580		Case-581		Case-582		Case-583		Case-584		Case-585		Case-586		Case-587		Case-588		Case-589		Case-590		Case-591		Case-592		Case-593		Case-594		Case-595		Case-596		Case-597		Case-598		Case-599		Case-600		Case-601		Case-602		Case-603		Case-604		Case-605		Case-606		Case-607		Case-608		Case-609		Case-610		Case-611		Case-612		Case-613		Case-614		Case-615		Case-616		Case-617		Case-618		Case-619		Case-620		Case-621		Case-622		Case-623		Case-624		Case-625		Case-626		Case-627		Case-628		Case-629		Case-630		Case-631		Case-632		Case-633		Case-634		Case-635		Case-636		Case-637		Case-638		Case-639		Case-640		Case-641		Case-642		Case-643		Case-644		Case-645		Case-646		Case-647		Case-648		Case-649		Case-650		Case-651		Case-652		Case-653		Case-654		Case-655		Case-656		Case-657		Case-658		Case-659		Case-660		Case-661		Case-662		Case-663		Case-664		Case-665		Case-666		Case-667		Case-668		Case-669		Case-670		Case-671		Case-672		Case-673		Case-674		Case-675		Case-676		Case-677		Case-678		Case-679		Case-680		Case-681		Case-682		Case-683		Case-684		Case-685		Case-686		Case-687		Case-688		Case-689		Case-690		Case-691		Case-692		Case-693		Case-694		Case-695		Case-696		Case-697		Case-698		Case-699		Case-700		Case-701		Case-702		Case-703		Case-704		Case-705		Case-706		Case-707		Case-708		Case-709		Case-710		Case-711		Case-712		Case-713		Case-714		Case-715		Case-716		Case-717		Case-718		Case-719		Case-720		Case-721		Case-722		Case-723		Case-724		Case-725		Case-726		Case-727		Case-728		Case-729		Case-730		Case-731		Case-732		Case-733		Case-734		Case-735		Case-736		Case-737		Case-738		Case-739		Case-740		Case-741		Case-742		Case-743		Case-744		Case-745		Case-746		Case-747		Case-748		Case-749		Case-750		Case-751		Case-752		Case-753		Case-754		Case-755		Case-756		Case-757		Case-758		Case-759		Case-760		Case-761		Case-762		Case-763		Case-764		Case-765		Case-766		Case-767		Case-768		Case-769		Case-770		Case-771		Case-772		Case-773		Case-774		Case-775		Case-776		Case-777		Case-778		Case-779		Case-780		Case-781		Case-782		Case-783		Case-784		Case-785		Case-786		Case-787		Case-788		Case-789		Case-790		Case-791		Case-792		Case-793		Case-794		Case-795		Case-796		Case-797		Case-798		Case-799		Case-800		Case-801		Case-802		Case-803		Case-804		Case-805		Case-806		Case-807		Case-808		Case-809		Case-810		Case-811		Case-812		Case-813		Case-814		Case-815		Case-816		Case-817		Case-818		Case-819		Case-820		Case-821		Case-822		Case-823		Case-824		Case-825		Case-826		Case-827		Case-828		Case-829		Case-830		Case-831		Case-832		Case-833		Case-834		Case-835		Case-836		Case-837		Case-838		Case-839		Case-840		Case-841		Case-842		Case-843		Case-844		Case-845		Case-846		Case-847		Case-848		Case-849		Case-850		Case-851		Case-852		Case-853		Case-854		Case-855		Case-856		Case-857		Case-858		Case-859		Case-860		Case-861		Case-862		Case-863		Case-864		Case-865		Case-866		Case-867		Case-868		Case-869		Case-870		Case-871		Case-872		Case-873		Case-874		Case-875		Case-876		Case-877		Case-878		Case-879		Case-880		Case-881		Case-882		Case-883		Case-884		Case-885		Case-886		Case-887		Case-888		Case-889		Case-890		Case-891		Case-892		Case-893		Case-894		Case-895		Case-896		Case-897		Case-898		Case-899		Case-900		Case-901		Case-902		Case-903		Case-904		Case-905		Case-906		Case-907		Case-908		Case-909		Case-910		Case-911		Case-912		Case-913		Case-914		Case-915		Case-916		Case-917		Case-918		Case-919		Case-920		Case-921		Case-922		Case-923		Case-924		Case-925		Case-926		Case-927		Case-928		Case-929		Case-930		Case-931		Case-932		Case-933		Case-934		Case-935		Case-936		Case-937		Case-938		Case-939		Case-940		Case-941		Case-942		Case-943		Case-944		Case-945		Case-946		Case-947		Case-948		Case-94	

Inlet (added component)		C7H14 with finite catalytic reaction rates at the wall (slow C7H14 rate = 10 x CH4 rate; moderate C7H14 rate = 2 x C3H8 rate)																									
		Case-1					Case-2					Case-3					Case-4					Case-5					
conc(ppm)		Recup-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s	Recup-m	600cpl-m	400cpl-s
5000	1.680	0.001005	1.7905	0.001005	0.005610	1.1508	0.001005	0.005610	1.1508	0.001005	0.005610	1.1508	0.001005	0.005610	1.1508	0.001005	0.005610	1.1508	0.001005	0.005610	1.1508	0.001005	0.005610	1.1508	0.001005	0.005610	1.1508
2000	0.4672	4.020E-04	0.7162	0.004672	0.014244	4.4690	0.004672	0.014244	4.4690	0.004672	0.014244	4.4690	0.004672	0.014244	4.4690	0.004672	0.014244	4.4690	0.004672	0.014244	4.4690	0.004672	0.014244	4.4690	0.004672	0.014244	4.4690
1000	0.2336	2.010E-04	0.3581	0.002336	0.007122	2.2345	0.002336	0.007122	2.2345	0.002336	0.007122	2.2345	0.002336	0.007122	2.2345	0.002336	0.007122	2.2345	0.002336	0.007122	2.2345	0.002336	0.007122	2.2345	0.002336	0.007122	2.2345
500	0.1168	1.005E-04	0.1791	0.001168	0.003561	1.1152	0.001168	0.003561	1.1152	0.001168	0.003561	1.1152	0.001168	0.003561	1.1152	0.001168	0.003561	1.1152	0.001168	0.003561	1.1152	0.001168	0.003561	1.1152	0.001168	0.003561	1.1152
200	0.04672	4.020E-05	0.07162	0.0004672	0.001424	0.4469	0.0004672	0.001424	0.4469	0.0004672	0.001424	0.4469	0.0004672	0.001424	0.4469	0.0004672	0.001424	0.4469	0.0004672	0.001424	0.4469	0.0004672	0.001424	0.4469	0.0004672	0.001424	0.4469
100	0.02336	2.010E-05	0.03581	0.0002336	0.000712	0.2234	0.0002336	0.000712	0.2234	0.0002336	0.000712	0.2234	0.0002336	0.000712	0.2234	0.0002336	0.000712	0.2234	0.0002336	0.000712	0.2234	0.0002336	0.000712	0.2234	0.0002336	0.000712	0.2234
50	0.01168	1.005E-05	0.01791	0.0001168	0.000356	0.1115	0.0001168	0.000356	0.1115	0.0001168	0.000356	0.1115	0.0001168	0.000356	0.1115	0.0001168	0.000356	0.1115	0.0001168	0.000356	0.1115	0.0001168	0.000356	0.1115	0.0001168	0.000356	0.1115
20	0.004672	4.020E-06	0.007162	0.00004672	0.0001424	0.04469	0.00004672	0.0001424	0.04469	0.00004672	0.0001424	0.04469	0.00004672	0.0001424	0.04469	0.00004672	0.0001424	0.04469	0.00004672	0.0001424	0.04469	0.00004672	0.0001424	0.04469	0.00004672	0.0001424	0.04469
10	0.002336	2.010E-06	0.003581	0.00002336	0.0000712	0.02234	0.00002336	0.0000712	0.02234	0.00002336	0.0000712	0.02234	0.00002336	0.0000712	0.02234	0.00002336	0.0000712	0.02234	0.00002336	0.0000712	0.02234	0.00002336	0.0000712	0.02234	0.00002336	0.0000712	0.02234
5	0.001168	1.005E-06	0.001791	0.00001168	0.0000356	0.01115	0.00001168	0.0000356	0.01115	0.00001168	0.0000356	0.01115	0.00001168	0.0000356	0.01115	0.00001168	0.0000356	0.01115	0.00001168	0.0000356	0.01115	0.00001168	0.0000356	0.01115	0.00001168	0.0000356	0.01115
2	0.0004672	4.020E-07	0.0003581	0.000004672	0.00001424	0.0004469	0.000004672	0.00001424	0.0004469	0.000004672	0.00001424	0.0004469	0.000004672	0.00001424	0.0004469	0.000004672	0.00001424	0.0004469	0.000004672	0.00001424	0.0004469	0.000004672	0.00001424	0.0004469	0.000004672	0.00001424	0.0004469
1	0.0002336	2.010E-07	0.0001791	0.000002336	0.00000712	0.0002234	0.000002336	0.00000712	0.0002234	0.000002336	0.00000712	0.0002234	0.000002336	0.00000712	0.0002234	0.000002336	0.00000712	0.0002234	0.000002336	0.00000712	0.0002234	0.000002336	0.00000712	0.0002234	0.000002336	0.00000712	0.0002234
C7H14 without reaction and CH4 with finite catalytic reaction rates at the wall		Case-1					Case-2					Case-3					Case-4					Case-5					
Inlet conc(ppm)		C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400	C7H14	CH4H400
5000	3.201E-04	318.00	381.30	0.012075	0.004050	708.80	0.004050	0.004050	708.80	0.004050	0.004050	708.80	0.004050	0.004050	708.80	0.004050	0.004050	708.80	0.004050	0.004050	708.80	0.004050	0.004050	708.80	0.004050	0.004050	708.80
2000	1.280E-04	124.00	156.52	0.004630	0.001420	282.20	0.001420	0.001420	282.20	0.001420	0.001420	282.20	0.001420	0.001420	282.20	0.001420	0.001420	282.20	0.001420	0.001420	282.20	0.001420	0.001420	282.20	0.001420	0.001420	282.20
1000	6.402E-05	62.0000	78.2600	0.002315	0.000710	141.10	0.000710	0.000710	141.10	0.000710	0.000710	141.10	0.000710	0.000710	141.10	0.000710	0.000710	141.10	0.000710	0.000710	141.10	0.000710	0.000710	141.10	0.000710	0.000710	141.10
500	3.201E-05	31.0000	39.1300	0.001158	0.000355	70.5500	0.000355	0.000355	70.5500	0.000355	0.000355	70.5500	0.000355	0.000355	70.5500	0.000355	0.000355	70.5500	0.000355	0.000355	70.5500	0.000355	0.000355	70.5500	0.000355	0.000355	70.5500
200	1.280E-05	12.4000	15.6520	0.000463	0.000142	28.2200	0.000142	0.000142	28.2200	0.000142	0.000142	28.2200	0.000142	0.000142	28.2200	0.000142	0.000142	28.2200	0.000142	0.000142	28.2200	0.000142	0.000142	28.2200	0.000142	0.000142	28.2200
100	6.402E-06	6.20000	7.82600	0.000231	0.000071	14.1100	0.000071	0.000071	14.1100	0.000071	0.000071	14.1100	0.000071	0.000071	14.1100	0.000071	0.000071	14.1100	0.000071	0.000071	14.1100	0.000071	0.000071	14.1100	0.000071	0.000071	14.1100
50	3.201E-06	3.10000	3.91300	0.000116	0.000036	7.05500	0.000036	0.000036	7.05500	0.000036	0.000036	7.05500	0.000036	0.000036	7.05500	0.000036	0.000036	7.05500	0.000036	0.000036	7.05500	0.000036	0.000036	7.05500	0.000036	0.000036	7.05500
20	1.280E-06	1.24000	1.56520	0.000046	0.000014	2.82200	0.000014	0.000014	2.82200	0.000014	0.000014	2.82200	0.000014	0.000014	2.82200	0.000014	0.000014	2.82200	0.000014	0.000014	2.82200	0.000014	0.000014	2.82200	0.000014	0.000014	2.82200
10	6.402E-07	0.62000	0.78260	0.000023	0.000007	0.70550	0.000007	0.000007	0.70550	0.000007	0.000007	0.70550	0.000007	0.000007	0.70550	0.000007	0.000007	0.70550	0.000007	0.000007	0.70550	0.000007	0.000007	0.70550	0.000007	0.000007	0.70550
5	3.201E-07	0.31000	0.39130	0.000012	0.000004	0.35275	0.000004	0.000004	0.35275	0.000004	0.000004	0.35275	0.000004	0.000004	0.35275	0.000004	0.000004	0.35275	0.000004	0.000004	0.35275	0.000004	0.000004	0.35275	0.000004	0.000004	0.35275
2	1.280E-07	0.12400	0.15652	0.000005	0.000002	0.14110	0.000002	0.000002	0.14110	0.000002	0.000002	0.14110	0.000002	0.000002	0.14110	0.000002	0.000002	0.14110	0.000002	0.000002	0.14110	0.000002	0.000002	0.14110	0.000002	0.000002	0.14110
1	6.402E-08	0.062000	0.078260	0.000002	0.000001	0.070550	0.000001	0.000001	0.070550	0.000001	0.000001	0.070550	0.000001	0.000001	0.070550	0.000001	0.000001	0.070550	0.000001	0.000001	0.070550	0.000001	0.000001	0.070550	0.000001	0.000001	0.070550
In(yout)/in																											
Case#:		1	2	3	4	5																					
C7H14Rs		2.34E-04	1.14E-03	2.67E-03	5.58E-03	3.60E-02																					
C7H14H600s		2.01E-07	7.12E-06	5.43E-05	2.99E-03	1.99E-02																					
C7H14H400s		3.58E-04	2.23E-03	6.34E-03	1.52E-02	1.46E-01																					
C7H14R		-16.56407	-12.93381	-10.86122	-9.1426817	-4.966427																					
CH4H600		0.062	0.118	0.1705	0.232	0.5693																					
CH4H400		0.07826	0.1411	0.1977	0.2621	0.5959																					

Gas Properties and Constants

cm = 0.01·m J = kg·m²·sec⁻² W = J·sec⁻¹ Pref = 1·atm
 N = kg·m·sec⁻² Pa = N·m⁻² atm = 101300·Pa μm = 0.000001·m
 R = 8.3143· $\frac{J}{K}$ Rc = 8.3143·J·mole⁻¹·K⁻¹

n	Gas	MolWt	σ(LJ)	ε(LJ)
0	CH4	MW ₀ = 16.044·gm	σ ₀ = 3.785·10 ⁻¹⁰ ·m	ε ₀ = 148.6·K
1	O2	MW ₁ = 31.999·gm	σ ₁ = 3.464·10 ⁻¹⁰ ·m	ε ₁ = 106.7·K
2	N2	MW ₂ = 28.018·gm	σ ₂ = 3.798·10 ⁻¹⁰ ·m	ε ₂ = 71.4·K
3	CO2	MW ₃ = 44.010·gm	σ ₃ = 3.941·10 ⁻¹⁰ ·m	ε ₃ = 195.2·K
4	H2O	MW ₄ = 18.015·gm	σ ₄ = 2.641·10 ⁻¹⁰ ·m	ε ₄ = 809.1·K
5	C7H14 methyl-cyclohexane		Tc7 = 572.2·K Tb7 = 374.1·K Pc7 = 3.47·10 ⁶ ·Pa Vc7 = 368	
			ε ₅ = $\frac{Tc7}{1.2593}$ σ ₅ = Vc7 ^{1/3} ·10 ⁻¹⁰ ·m	
		MW ₅ = 98.189·gm	σ ₅ = 7.1661·10 ⁻¹⁰ ·m	ε ₅ = 454.3794·K
6	CO	MW ₆ = 28.01·gm	σ ₆ = 3.69·10 ⁻¹⁰ ·m	ε ₆ = 91.7·K

Define constants for transport integrals:

σμa ₀ = 1.16145	σμb ₀ = 0.14874	σDa ₀ = 1.06036	σDb ₀ = 0.1561
σμa ₁ = 0.52487	σμb ₁ = 0.7732	σDa ₁ = 0.193	σDb ₁ = 0.47635
σμa ₂ = 2.16178	σμb ₂ = 2.43787	σDa ₂ = 1.03587	σDb ₂ = 1.52996
		σDa ₃ = 1.76474	σDb ₃ = 3.89411

Define transport integrals:

$$\Omega\mu(T) = \sigma\mu a_0 \cdot \exp\left[-\frac{\sigma\mu b_0}{T}\right] + \sum_{i\mu=1}^2 \sigma\mu a_{i\mu} \cdot \exp\left[-\frac{\sigma\mu b_{i\mu}}{T}\right] \quad \Omega\mu(3) = 1.0394$$

$$\Omega D(T) = \sigma D a_0 \cdot \exp\left[-\frac{\sigma D b_0}{T}\right] + \sum_{i\mu=1}^3 \sigma D a_{i\mu} \cdot \exp\left[-\frac{\sigma D b_{i\mu}}{T}\right] \quad \Omega D(3) = 0.95002$$

Set Inlet Conditions:

$$P = 1 \text{ atm}$$

$$\phi = 0.1$$

$$y_{adc7} = 0.0021859$$

This value for y_{adc7} was determined via enthalpy functions [REDACTED] for temperature rise from 1000F to 1511F.

$$y_{eqc7} = \phi \frac{0.205}{14}$$

$$\phi_{eq} = \phi \frac{y_{adc7}}{y_{eqc7}}$$

The value for y_{eq} was determined for a given equivalence ratio of 0.1 in moist air

$$y_{eqc7} = 0.001464$$

$$\phi_{eq} = 0.149281$$

Define gas composition with C7H14 fuel using moist (2%) air:

$$y_7(y_0, x) = \frac{\begin{bmatrix} 0 \\ (1 - y_0) \cdot 0.205 - 10.5 \cdot y_0 \cdot x \\ (1 - y_0) \cdot 0.775 \\ 7 \cdot (y_0 \cdot x) \\ (1 - y_0) \cdot 0.02 + 7 \cdot y_0 \cdot x \\ y_0 \cdot (1 - x) \\ 0 \end{bmatrix}}{1 + 2.5 \cdot y_0 \cdot x}$$

$$y_{eq} := y_7(y_{eqc7}, 1)$$

$$y_{ad} := y_7(y_{adc7}, 1)$$

$$y_{eq} = \begin{bmatrix} 0 \\ 0.188634 \\ 0.771043 \\ 0.010213 \\ 0.03011 \\ 0 \\ 0 \end{bmatrix}$$

$$y_{ad} = \begin{bmatrix} 0 \\ 0.180613 \\ 0.769103 \\ 0.015218 \\ 0.035066 \\ 0 \\ 0 \end{bmatrix}$$

Define functions for evaluation of mixture properties (ideal gas) for complete fuel conversion and a given temperature.

Density and average molecular weight:

$$\rho_{mix}(T) = \sum_{kk=0}^6 y_{eq_{kk}} \cdot MW_{kk} \cdot \frac{P}{R \cdot T}$$

$$MW_{mix} = \sum_{kk=0}^6 y_{eq_{kk}} \cdot MW_{kk}$$

$$\rho_{mix}(300 \cdot K) = 1.162787 \cdot \text{kg} \cdot \text{m}^{-3}$$

$$MW_{mix} = 28.631 \cdot \text{gm}$$

Define diffusion coefficients for specific binary diffusion pairs:

$$\text{Diff}(n,m,T) = 1.8829 \cdot 10^{-27} \cdot \left[\frac{1}{\text{MW}_n} + \frac{1}{\text{MW}_m} \right] \cdot T^{3/2} \cdot 10^8 \cdot \text{gm}^{0.5} \cdot \text{cm}^4 \cdot \text{sec}^{-1} \cdot \text{K}^{-1.5} \cdot \left(\frac{\sigma_n + \sigma_m}{2} \right)^2 \cdot \Omega_D \left[\frac{T}{\epsilon_n \cdot \epsilon_m} \right]^{0.5} \cdot \frac{P}{P_{\text{ref}}}$$

$$\text{Diff}(0,2,300\text{-K}) = 0.2225 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\text{Diff}(2,6,300\text{-K}) = 0.207 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define functions for use with various fuel-air mixtures:

$$D_{\text{ch4}}(T) = \frac{1}{\sum_{j_{\text{gas}}=1}^4 \frac{y_{\text{eq}_{j_{\text{gas}}}}}{\text{Diff}(0,j_{\text{gas}},T)}}$$

$$D_{\text{ch4}}(298\text{-K}) = 2.1912 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$D_{\text{c7h14}}(T) = \frac{1}{\sum_{j_{\text{gas}}=1}^4 \frac{y_{\text{eq}_{j_{\text{gas}}}}}{\text{Diff}(5,j_{\text{gas}},T)}}$$

$$D_{\text{c7h14}}(298\text{-K}) = 5.8372 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$D_{\text{co}}(T) = \frac{1}{\sum_{j_{\text{gas}}=1}^4 \frac{y_{\text{eq}_{j_{\text{gas}}}}}{\text{Diff}(6,j_{\text{gas}},T)}}$$

$$D_{\text{co}}(298\text{-K}) = 2.0451 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

Display gas mixture properties

idsp 0..9

$$T_{\text{in}} = \left[(1000 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K}$$

$$T_{\text{in}} = 810.9278 \cdot \text{K}$$

$$T_{\text{dsp}_{\text{idsp}}} = (750 + 50 \cdot \text{idsp}) \cdot \text{K}$$

$$T_{\text{out}} = \left[(1511 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K}$$

$$T_{\text{out}} = 1094.8167 \cdot \text{K}$$

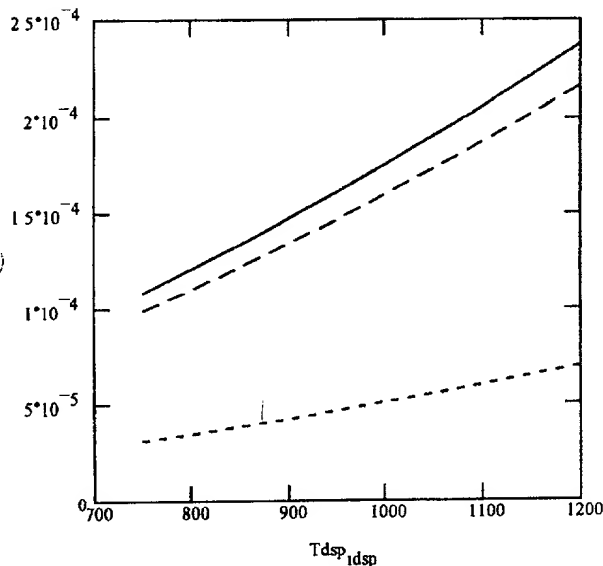


TABLE 5.1

Tdsp _{idsp}	Dch4(Tdsp _{idsp})	Dc7h14(Tdsp _{idsp})	Dco(Tdsp _{idsp})
7.5·10 ² ·K	1.082·10 ⁻⁴ ·m ² ·sec ⁻¹	3.1097·10 ⁻⁵ ·m ² ·sec ⁻¹	9.8836·10 ⁻⁵ ·m ² ·sec ⁻¹
8·10 ² ·K	1.2064·10 ⁻⁴ ·m ² ·sec ⁻¹	3.4776·10 ⁻⁵ ·m ² ·sec ⁻¹	1.101·10 ⁻⁴ ·m ² ·sec ⁻¹
8.5·10 ² ·K	1.3359·10 ⁻⁴ ·m ² ·sec ⁻¹	3.8613·10 ⁻⁵ ·m ² ·sec ⁻¹	1.2184·10 ⁻⁴ ·m ² ·sec ⁻¹
9·10 ² ·K	1.4705·10 ⁻⁴ ·m ² ·sec ⁻¹	4.2603·10 ⁻⁵ ·m ² ·sec ⁻¹	1.3402·10 ⁻⁴ ·m ² ·sec ⁻¹
9.5·10 ² ·K	1.61·10 ⁻⁴ ·m ² ·sec ⁻¹	4.6743·10 ⁻⁵ ·m ² ·sec ⁻¹	1.4665·10 ⁻⁴ ·m ² ·sec ⁻¹
1·10 ³ ·K	1.7543·10 ⁻⁴ ·m ² ·sec ⁻¹	5.1031·10 ⁻⁵ ·m ² ·sec ⁻¹	1.5972·10 ⁻⁴ ·m ² ·sec ⁻¹
1.05·10 ³ ·K	1.9033·10 ⁻⁴ ·m ² ·sec ⁻¹	5.5462·10 ⁻⁵ ·m ² ·sec ⁻¹	1.7322·10 ⁻⁴ ·m ² ·sec ⁻¹
1.1·10 ³ ·K	2.057·10 ⁻⁴ ·m ² ·sec ⁻¹	6.0035·10 ⁻⁵ ·m ² ·sec ⁻¹	1.8714·10 ⁻⁴ ·m ² ·sec ⁻¹
1.15·10 ³ ·K	2.2152·10 ⁻⁴ ·m ² ·sec ⁻¹	6.4746·10 ⁻⁵ ·m ² ·sec ⁻¹	2.0148·10 ⁻⁴ ·m ² ·sec ⁻¹
1.2·10 ³ ·K	2.378·10 ⁻⁴ ·m ² ·sec ⁻¹	6.9593·10 ⁻⁵ ·m ² ·sec ⁻¹	2.1624·10 ⁻⁴ ·m ² ·sec ⁻¹

Define interpolation formulas for Dch4, Dc7h14, and Dco vs. T(K) via Jandel Scientific's Tablecurve program

$$Dch4T(T) = \exp\left(-10.623294 + 1.6259688 \cdot \ln\left(\frac{T}{K}\right) - \frac{46.41736 \cdot K}{T}\right) \cdot \frac{cm^2}{sec}$$

$$Dch4(1000 \cdot K) = 1.75426 \cdot sec^{-1} \cdot cm^2$$

$$Dch4T(1000 \cdot K) = 1.75432 \cdot sec^{-1} \cdot cm^2$$

$$Dc7h14T(T) = \exp\left(11.822189 + 1.6260138 \cdot \ln\left(\frac{T}{K}\right) - \frac{82.65375 \cdot K}{T}\right) \cdot \frac{cm^2}{sec}$$

$$Dc7h14(1000 \cdot K) = 0.51031 \cdot sec^{-1} \cdot cm^2$$

$$Dc7h14T(1000 \cdot K) = 0.51031 \cdot sec^{-1} \cdot cm^2$$

$$DcoT(T) = \exp\left(10.831955 + 1.6394196 \cdot \ln\left(\frac{T}{K}\right) - \frac{24.53899 \cdot K}{T}\right) \cdot \frac{cm^2}{sec}$$

$$Dco(1000 \cdot K) = 1.59722 \cdot sec^{-1} \cdot cm^2$$

$$DcoT(1000 \cdot K) = 1.59714 \cdot sec^{-1} \cdot cm^2$$

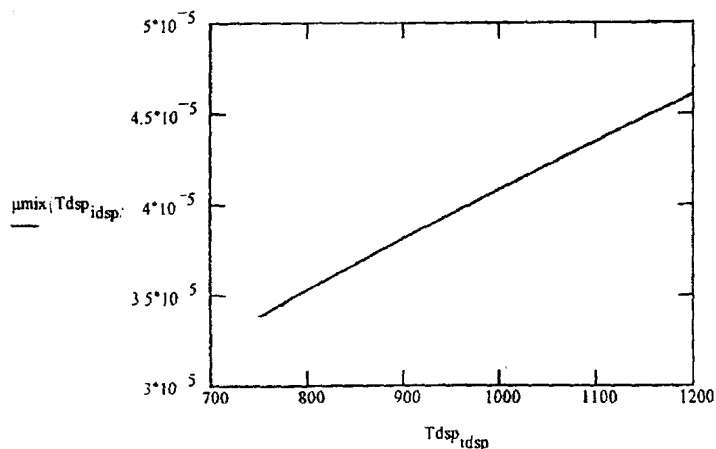
Define viscosity functions for major constituents:

$$\mu(T) = \frac{2.6693 \cdot 10^{-26} \cdot \left(\frac{MW_0 \cdot T}{(\sigma_0)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_0} \right)} \right)^{0.5} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5}}{\left(\frac{MW_1 \cdot T}{\sigma_1^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_1} \right)} \right)^{0.5} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right]} \\ + \frac{\left(\frac{MW_2 \cdot T}{\sigma_2^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_2} \right)} \right)^{0.5} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right]}{\left(\frac{MW_3 \cdot T}{\sigma_3^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_3} \right)} \right)^{0.5} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right]} \\ + \frac{1.116 \cdot \left(\frac{MW_4 \cdot T}{(3.115 \cdot 10^{-8} \cdot \text{cm})^2 \cdot \Omega \mu \left(\frac{T}{514 \cdot \text{K}} \right)} \right)^{0.5} \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right]}{\left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right]}$$

$$\mu(300 \cdot \text{K}) = \begin{bmatrix} 1.10281 \cdot 10^{-5} \\ 2.0603 \cdot 10^{-5} \\ 1.76981 \cdot 10^{-5} \\ 1.51851 \cdot 10^{-5} \\ 1.06784 \cdot 10^{-5} \end{bmatrix} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(T) = \sum_{n=1}^4 \frac{y_{\text{eq}_n} \cdot \mu(T)_n}{\sum_{m=1}^4 y_{\text{eq}_m} \cdot \left[\frac{1 + \left(\frac{\mu(T)_n}{\mu(T)_m} \right)^{0.5} \cdot \left(\frac{MW_m}{MW_n} \right)^{0.25} \right]^2} \cdot \left[8 \cdot \left(1 + \frac{MW_n}{MW_m} \right) \right]^{0.5}}$$

$$y_{\text{eq}} = \begin{bmatrix} 0 \\ 0.1886 \\ 0.771 \\ 0.0102 \\ 0.0301 \\ 0 \\ 0 \end{bmatrix}$$



$T_{\text{dsp_idsp}}$
750-K
800-K
850-K
900-K
950-K
1000-K
1050-K
1100-K
1150-K
1200-K

$\mu_{\text{mix}}(T_{\text{dsp_idsp}})$
$3.3875 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.5348 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.6787 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.8194 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$3.9573 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.0926 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.2254 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.356 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.4844 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$
$4.6108 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$

$$\mu_{\text{mix}}(T) = \exp \left[-0.6984944 + 0.640549 \cdot \ln \left(\frac{T}{K} \right) + \frac{-14.50559 \cdot K}{T} \right] \cdot 10^{-6} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(1000 \cdot K) = 4.0926 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

$$\mu_{\text{mix}}(1000 \cdot K) = 4.09256 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

Define thermal conductivity functions for light molecules

igas = 0, 1..4

$$a\lambda = \begin{bmatrix} -1.869 \\ -3.273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda = \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda = \begin{bmatrix} 1.179 \cdot 10^{-4} \\ -(3.743 \cdot 10^{-5}) \\ -(5.067 \cdot 10^{-5}) \\ 5.477 \cdot 10^{-6} \\ 1.801 \cdot 10^{-4} \end{bmatrix}$$

$$d\lambda = \begin{bmatrix} -(3.614 \cdot 10^{-8}) \\ 9.732 \cdot 10^{-9} \\ 1.504 \cdot 10^{-8} \\ -(1.053 \cdot 10^{-8}) \\ -(9.1 \cdot 10^{-8}) \end{bmatrix}$$

CH4
O2
N2
CO2
H2O

$$\lambda(i, T) = \left[a\lambda_i + b\lambda_i \cdot \frac{T}{K} + c\lambda_i \cdot \left(\frac{T}{K} \right)^2 + d\lambda_i \cdot \left(\frac{T}{K} \right)^3 \right] \cdot 0.00001 \cdot \frac{W}{\text{cm} \cdot K}$$

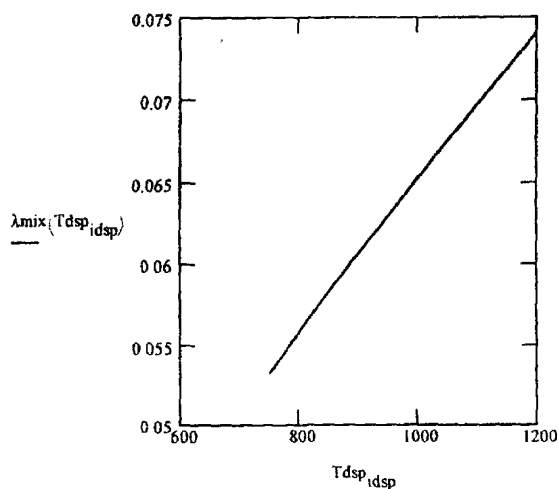
$\lambda(\text{igas}, 1000 \cdot K)$

0.16716 · kg · m · sec ⁻³ · K ⁻¹
0.07163 · kg · m · sec ⁻³ · K ⁻¹
0.06292 · kg · m · sec ⁻³ · K ⁻¹
0.06788 · kg · m · sec ⁻³ · K ⁻¹
0.08631 · kg · m · sec ⁻³ · K ⁻¹

W/m/K

$$\lambda_{\text{mix}}(T) = \sum_{i=1}^4 \frac{y_{eq,i} \cdot \lambda(i, T)}{\sum_{j=1}^4 y_{eq,j} \cdot \left[\frac{1 + \left(\frac{\mu(T)_i}{\mu(T)_j} \right)^{0.5} \cdot \left(\frac{MW_j}{MW_i} \right)^{0.25} \right]^2} \cdot \left[8 \cdot \left(1 + \frac{MW_j}{MW_i} \right) \right]^{0.5}}$$

$$\lambda_{\text{mix}}(1000 \cdot K) = 0.000653 \cdot \frac{W}{\text{cm} \cdot K}$$



$T_{\text{dsp_idsp}}$	$\lambda_{\text{mix}}(T_{\text{dsp_idsp}})$
7.5 · 10 ² · K	0.05323 · kg · m · sec ⁻³ · K ⁻¹
8 · 10 ² · K	0.055775 · kg · m · sec ⁻³ · K ⁻¹
8.5 · 10 ² · K	0.058242 · kg · m · sec ⁻³ · K ⁻¹
9 · 10 ² · K	0.060641 · kg · m · sec ⁻³ · K ⁻¹
9.5 · 10 ² · K	0.06298 · kg · m · sec ⁻³ · K ⁻¹
1 · 10 ³ · K	0.065268 · kg · m · sec ⁻³ · K ⁻¹
1.05 · 10 ³ · K	0.067512 · kg · m · sec ⁻³ · K ⁻¹
1.1 · 10 ³ · K	0.069721 · kg · m · sec ⁻³ · K ⁻¹
1.15 · 10 ³ · K	0.071904 · kg · m · sec ⁻³ · K ⁻¹
1.2 · 10 ³ · K	0.074069 · kg · m · sec ⁻³ · K ⁻¹

$$\lambda_{\text{mix}}T(T) = \exp\left[-7.073383 + 0.6397005 \cdot \ln\left(\frac{T}{K}\right) + \frac{65.2387 \cdot K}{T}\right] \cdot W \cdot m^{-1} \cdot K^{-1}$$

$$\lambda_{\text{mix}}(1000 \cdot K) = 0.0653 \cdot m^{-1} \cdot K^{-1} \cdot W$$

$$\lambda_{\text{mix}}T(1000 \cdot K) = 0.0659 \cdot m^{-1} \cdot K^{-1} \cdot W$$

Define heat capacities:

$$Cp_{\text{coef}} = \begin{bmatrix} 19.25 & .05213 & 0.00001197 & -0.00000001132 \\ 28.11 & -0.000368 & 0.00001746 & -0.00000001065 \\ 31.15 & -0.01357 & 0.0000268 & -0.00000001168 \\ 19.8 & 0.07344 & -0.00005602 & 0.00000001715 \\ 32.24 & 0.001924 & 0.00001055 & -0.000000003596 \\ 76.19 & 0.7867 & -0.0004204 & 0.00000007516 \end{bmatrix}$$

$$Cp(\text{igas}, T) = \sum_{jj=0}^3 Cp_{\text{coef}}_{\text{igas}, jj} \cdot \left(\frac{T}{K}\right)^{jj} \cdot \frac{J}{K}$$

J/mol/K

$$jj = 0..3$$

$$Cp(0, 300 \cdot K) = 35.6607 \cdot K^{-1} \cdot J$$

$$Cp(5, 300 \cdot K) = 124.0133 \cdot K^{-1} \cdot J$$

$$Cp_{\text{mix}}(T) = \sum_{jk=1}^4 Cp(jk, T) \cdot yeq_{jk}$$

$$Cp_{\text{mix}}(998 \cdot K) = 33.5144 \cdot J \cdot K^{-1}$$

$$Cp_{\text{cfmix}}_{jj} = \sum_{jk=1}^4 Cp_{\text{coef}}_{jk, jj} \cdot yeq_{jk} \cdot \frac{J}{K}$$

$$Cp_{\text{cfmix}} = \begin{bmatrix} 30.493459 \\ -0.009725 \\ 2.370305 \cdot 10^{-5} \\ -1.094786 \cdot 10^{-8} \end{bmatrix} \cdot \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} \cdot \text{J}$$

$$Cp_{\text{mix}}T(T) = \sum_{jj=0}^3 Cp_{\text{cfmix}}_{jj} \cdot \left(\frac{T}{K}\right)^{jj}$$

$$Cp_{\text{mix}}(1000 \cdot K) = 33.52413 \cdot \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} \cdot K^{-1}$$

$$Cp_{\text{mix}}T(1000 \cdot K) = 33.52413 \cdot \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} \cdot K^{-1}$$

$$\text{igas} = 0, 1..6$$

$$P = 1.013 \cdot 10^5 \cdot \text{Pa}$$

 Define momentum and thermal diffusivities:

$$\alpha(\text{igas}, T) := \frac{\lambda(\text{igas}, T) \cdot R \cdot T}{Cp(\text{igas}, T) \cdot P}$$

$$\alpha(0, 300 \cdot K) = 0.2344 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\alpha_{\text{mix}}(T) := \frac{\lambda_{\text{mix}}(T) \cdot R \cdot T}{Cp_{\text{mix}}(T) \cdot P}$$

$$\alpha_{\text{mix}}(1000 \cdot K) = 1.6132 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\nu_{\text{mix}}(T) := \frac{\mu_{\text{mix}}(T)}{\rho_{\text{mix}}(T)}$$

$$\nu_{\text{mix}}(1000 \cdot K) = 1.1732 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\nu_{\text{mix}}(T) := \frac{\mu_{\text{mix}}(T)}{\rho_{\text{mix}}(T)}$$

$$\rho_{\text{mix}}(1000 \cdot K) = 3.48836 \cdot 10^{-4} \cdot \text{gm} \cdot \text{cm}^{-3}$$

$$\rho_{\text{mix}}(T) = \rho_{\text{mix}}(T)$$

$$D_{\text{ch4T}}(1000 \cdot K) = 1.7543 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c7h14T}}(1000 \cdot K) = 0.5103 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define Prandl, Schmidt, and Lewis numbers

$$Pr(T) := \frac{\nu_{\text{mix}}(T)}{\alpha_{\text{mix}}(T)}$$

$$Pr(1000 \cdot K) = 0.7272$$

$$Sc1T(T) := \frac{\nu_{\text{mix}}(T)}{D_{\text{ch4T}}(T)}$$

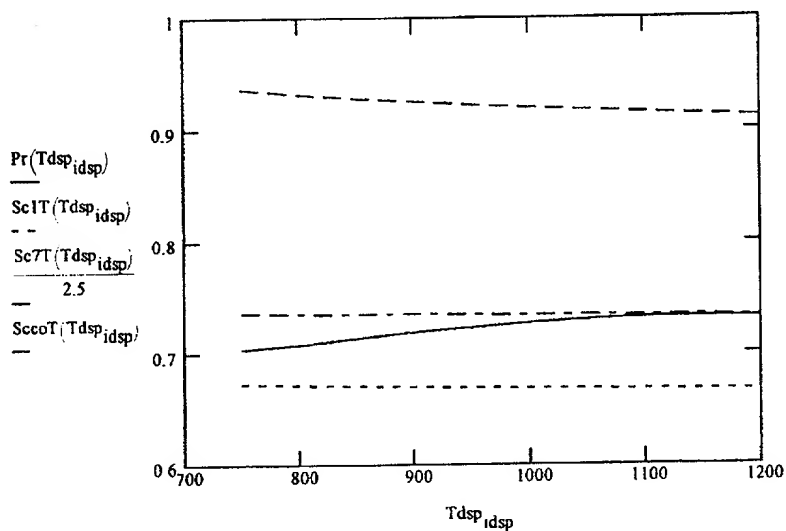
$$Sc1T(1000 \cdot K) = 0.6688$$

$$Sc7T(T) := \frac{\nu_{\text{mix}}(T)}{D_{\text{c7h14T}}(T)}$$

$$Sc7T(1000 \cdot K) = 2.299$$

$$SccoT(T) := \frac{\nu_{\text{mix}}(T)}{D_{\text{coT}}(T)}$$

$$SccoT(1000 \cdot K) = 0.7346$$



These relations have weak temperature dependence and (presumably) very weak dependence on composition

This ends the extended section that defines gas properties for the combustion mixtures.

Honeycombs: Represent as square channel metal alloy wall 0.003 mil, uncoated; 0.004 mil coated

$$dwalluc = 0.003 \cdot \text{in} \quad dwalluc = 7.62 \cdot 10^{-5} \cdot \text{m} \quad dwallc = 0.004 \cdot \text{in} \quad dwallc = 1.016 \cdot 10^{-4} \cdot \text{m}$$

$$\text{Cells1} = 100 \cdot \text{in}^{-2} \quad dwall1 = dwallc \quad \text{Cells2} = 200 \cdot \text{in}^{-2} \quad dwall2 = dwallc$$

$$dcell1 = (\text{Cells1})^{-0.5} \cdot dwall1 \quad dcell2 = (\text{Cells2})^{-0.5} \cdot dwall2$$

$$dcell1 = 0.2438 \cdot \text{cm} \quad ks1 = 0.002 \cdot \text{cm} \quad dcell2 = 0.1694 \cdot \text{cm} \quad ks2 = 0.002 \cdot \text{cm}$$

$$\epsilon_{cell1} = dcell1^2 \cdot \text{Cells1} \quad \epsilon_{cell1} = 0.9216 \quad \epsilon_{cell2} = dcell2^2 \cdot \text{Cells2} \quad \epsilon_{cell2} = 0.89006$$

$$\text{Cells4} = 400 \cdot \text{in}^{-2} \quad dwall4 = dwallc$$

$$\text{Cells6} = 600 \cdot \text{in}^{-2} \quad dwall6 = dwalluc$$

$$dcell4 = (\text{Cells4})^{-0.5} \cdot dwall4 \quad dcell4 = 0.1168 \cdot \text{cm}$$

$$dcell6 = (\text{Cells6})^{-0.5} \cdot dwall6 \quad dcell6 = 0.0961 \cdot \text{cm}$$

$$dcell4 = 0.1168 \cdot \text{cm} \quad ks4 = 0.001 \cdot \text{cm}$$

$$dcell6 = 0.0961 \cdot \text{cm} \quad ks6 = 0 \cdot \text{cm}$$

$$\epsilon_{cell4} = dcell4^2 \cdot \text{Cells4} \quad \epsilon_{cell4} = 0.8464$$

$$\epsilon_{cell6} = dcell6^2 \cdot \text{Cells6} \quad \epsilon_{cell6} = 0.85843$$

$$\text{Cells8} = 800 \cdot \text{in}^{-2} \quad dwall8 = dwalluc$$

$$dcell8 = (\text{Cells8})^{-0.5} \cdot dwall8 \quad dcell8 = 0.0822 \cdot \text{cm}$$

$$dcell8 = 0.0822 \cdot \text{cm} \quad ks8 = 0 \cdot \text{cm}$$

$$\epsilon_{cell8} = dcell8^2 \cdot \text{Cells8} \quad \epsilon_{cell8} = 0.83749$$

Define recuperator and monolith configurations:

$$dreco = 17 \cdot \text{in}$$

$$dreco = 43.18 \cdot \text{cm}$$

$$Lrec = 7 \cdot \text{in}$$

$$dreci = 6 \cdot \text{in}$$

$$dreci = 15.24 \cdot \text{cm}$$

$$Lrec = 17.78 \cdot \text{cm}$$

$$\delta d = 1.375 \cdot \text{in}$$

Add space for mounting and insulation?

$$dhco = dreco - \delta d$$

$$dhco = 39.6875 \cdot \text{cm}$$

$$Lhc = 4 \cdot \text{in}$$

$$dhci = dreci + \delta d$$

$$dhci = 18.7325 \cdot \text{cm}$$

$$Lhc = 10.16 \cdot \text{cm}$$

$$Shc = \pi \cdot \frac{dhco^2 - dhci^2}{4}$$

$$Shc = 0.0961 \cdot \text{m}^2$$

$$Srecup = 0.0958 \cdot \text{m}^2$$

$$\frac{Srecup}{Shc} = 0.9964$$

Define initial combustion conditions

$$jcase = 0, 1, 4$$

	0.2	1350	340
	0.26	1350	390
case	0.314	1350	440
	0.38	1350	490
	0.72	1190	675

Mass flow (lb/sec)
Recup T inlet (F)
Recup T outlet (F)

$$TKF(T) = \left(\frac{T}{K} - 273.15 \right) \cdot \frac{9}{5} + 32$$

$$TFK(t) = \left(\left(\frac{t}{9} - 32 \right) \cdot 5 \right) \cdot K + 273.15 \cdot K$$

$$P_{rec} = 1 \cdot \text{atm}$$

$$P_{hc} = 1 \cdot \text{atm}$$

$$mf_{jcase+1} = case_{jcase,0} \cdot 0.454 \cdot \text{kg} \cdot \text{sec}^{-1}$$

$$T_{recin_{jcase+1}} = TFK(case_{jcase,1})$$

$$T_{recout_{jcase+1}} = TFK(case_{jcase,2})$$

$$mf = \begin{bmatrix} 0 \\ 0.0908 \\ 0.118 \\ 0.1426 \\ 0.1725 \\ 0.3269 \end{bmatrix} \cdot \text{kg} \cdot \text{sec}^{-1}$$

$$T_{recin} = \begin{bmatrix} 0 \\ 1005.37 \\ 1005.37 \\ 1005.37 \\ 1005.37 \\ 916.48 \end{bmatrix} \cdot \text{K}$$

$$T_{recout} = \begin{bmatrix} 0 \\ 444.26 \\ 472.04 \\ 499.82 \\ 527.59 \\ 630.37 \end{bmatrix} \cdot \text{K}$$

$$U_{rec_{jcase+1}} = \frac{mf_{jcase+1}}{\rho_{mix}(T_{recin_{jcase+1}}) \cdot \frac{S_{recup}}{2}}$$

$$U_{rec} = \begin{bmatrix} 0 \\ 5.4633 \\ 7.1023 \\ 8.5774 \\ 10.3803 \\ 17.929 \end{bmatrix} \cdot \text{m} \cdot \text{sec}^{-1}$$

$$G_{rec_{jcase+1}} = \frac{mf_{jcase+1}}{\left(\frac{S_{recup}}{2}\right)}$$

Only half of the recuperator cross section
is available for exhaust gas flow

$$U_{hc2_{jcase+1}} = \frac{mf_{jcase+1}}{\rho_{mix}(T_{recin_{jcase+1}}) \cdot Shc \cdot \varepsilon_{cell2}}$$

$$U_{hc4_{jcase+1}} = U_{hc2_{jcase+1}} \cdot \frac{\varepsilon_{cell2}}{\varepsilon_{cell4}}$$

$$U_{hc6_{jcase+1}} = U_{hc2_{jcase+1}} \cdot \frac{\varepsilon_{cell2}}{\varepsilon_{cell6}}$$

$$U_{hc2} = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot \text{m} \cdot \text{sec}^{-1}$$

$$U_{hc4} = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot \text{m} \cdot \text{sec}^{-1}$$

$$T_{avg} = \frac{T_{recin} + T_{recout}}{2}$$

$$T_{avg} = \begin{bmatrix} 0 \\ 724.8167 \\ 738.7056 \\ 752.5944 \\ 766.4833 \\ 773.4278 \end{bmatrix} \cdot \text{K}$$

Define average temperature etc/ for
estimated ΔP and ΔT in the recuperator

$$\rho_{mixrec}(T) = \frac{MW_{mix} \cdot P_{rec}}{R \cdot T}$$

$$\rho_{mixrec}(T_{avg_1}) = 0.4813 \cdot \text{kg} \cdot \text{m}^{-3}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$R_{rec6}(G, T) = \frac{G \cdot d_{cell6}}{\mu_{mixT}(T)} \quad R_{rec6}(G_{rec1}, T_{avg1}) = 54.9906$$

$$R_{rec8}(G, T) = \frac{G \cdot d_{cell8}}{\mu_{mixT}(T)} \quad R_{rec8}(G_{rec1}, T_{avg1}) = 47.0389$$

For laminar flow with entrance effect (adapted from Kays & Crawford, "Convective Heat and Mass Transfer"):

$$c_{frec8}(G, T, z) = \frac{14.227}{R_{rec8}(G, T)} \left[1 + 0.046263 \cdot \left(R_{rec8}(G, T) \cdot \frac{d_{cell8}}{z} \right) \right]^{0.45363}$$

Average coefficient of friction
for a smooth square channel

$$c_{frec6}(G, T, z) = \frac{14.227}{R_{rec6}(G, T)} \left[1 + 0.046263 \cdot \left(R_{rec6}(G, T) \cdot \frac{d_{cell6}}{z} \right) \right]^{0.45363}$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta P_{rec8, j_{case}+1} = 4 \cdot c_{frec8}(G_{rec, j_{case}+1}, T_{avg, j_{case}+1}, L_{rec}) \cdot \frac{\left(\frac{U_{rec, j_{case}+1}}{2} \right)^2 \left[\rho_{mixrec}(T_{recin, j_{case}+1}) + \rho_{mixrec}(T_{recout, j_{case}+1}) \right] \cdot \left(\frac{T_{recin}}{T_{rec}} \right)}{2}$$

$$\Delta P_{rec6, j_{case}+1} = 4 \cdot c_{frec6}(G_{rec, j_{case}+1}, T_{avg, j_{case}+1}, L_{rec}) \cdot \frac{\left(\frac{U_{rec, j_{case}+1}}{2} \right)^2 \left[\rho_{mixrec}(T_{recin, j_{case}+1}) + \rho_{mixrec}(T_{recout, j_{case}+1}) \right] \cdot \left(\frac{T_{recin}}{T_{rec}} \right)}{2}$$

$$\frac{\Delta P_{rec8}}{Prec} = \begin{bmatrix} 0 \\ 0.0097 \\ 0.013 \\ 0.0162 \\ 0.0203 \\ 0.0393 \end{bmatrix}$$

$$\frac{\Delta P_{rec6}}{Prec} = \begin{bmatrix} 0 \\ 0.0071 \\ 0.0095 \\ 0.0119 \\ 0.0149 \\ 0.0289 \end{bmatrix}$$

$$\Delta P_{obs_P} = \begin{bmatrix} 0 \\ 0.011 \\ 0.014 \\ 0.018 \\ 0.022 \\ 0.042 \end{bmatrix}$$

Chose 800 cells per in2
with 10% length factor
in Lrec for chevrons

Averaged Nu for 800 cpi square channels (fully developed laminar flow) taken from Rosner:

$$\text{Nuhavgrec8}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left[\frac{7.6 \cdot (\text{Lrec} \cdot 1.1)}{\text{Rerec8}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Pr}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dcell8}} \right] \right]^{\frac{1}{8}}$$

$$\text{Nuhavgrec8} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.976 \\ 2.976 \\ 2.9762 \end{bmatrix}$$

Entrance effect for heat transfer within the recuperator is only significant for the first half inch - average Nusselt No. = 2.976 for all cases

$$\text{hrecavg}_{j\text{case}+1} = \frac{\lambda_{\text{mix}}(\text{Tavg}_{j\text{case}+1}) \cdot \text{Nuhavgrec8}_{j\text{case}+1}}{\text{dcell8}}$$

$$\text{hrecavg} = \begin{bmatrix} 0 \\ 188.0022 \\ 190.6356 \\ 193.2448 \\ 195.8307 \\ 197.1273 \end{bmatrix} \cdot \text{kg} \cdot \text{sec}^{-3} \cdot \text{K}^{-1}$$

W/m2/K

$$\Delta T_{\text{skin}}_{j\text{case}+1} = \frac{\text{Grec}_{j\text{case}+1} \cdot \text{dcell8} \cdot (\text{Cpmix}(\text{Trecout}_{j\text{case}+1}) \cdot \text{Trecout}_{j\text{case}+1} - \text{Cpmix}(\text{Trecin}_{j\text{case}+1}) \cdot \text{Trecin}_{j\text{case}+1})}{\text{MWmix} \cdot \text{hrecavg}_{j\text{case}+1} \cdot 4 \cdot \text{Lrec} \cdot 1.1}$$

$$\Delta T_{\text{skin}} = \begin{bmatrix} 0 \\ -7.5657 \\ -9.274 \\ -10.5339 \\ -11.9549 \\ -13.635 \end{bmatrix} \cdot \text{K}$$

$$\Delta T_{\text{skin}} \cdot 2 \cdot \frac{9}{5 \cdot \text{K}} = \begin{bmatrix} 0 \\ -27.2364 \\ -33.3864 \\ -37.9221 \\ -43.0378 \\ -49.0859 \end{bmatrix}$$

Approximate average ΔT (F)
across wall in recuperator

ΔT seems low - more conservative calculation uses dcell for 600 cells/in2 - in this case ΔT maximum increases from 50F to about 70F

$$\Delta T_{\text{skin}} \cdot 2 \cdot \frac{9}{5 \cdot \text{K}} \cdot \left(\frac{\text{dcell6}}{\text{dcell8}} \right)^2 = \begin{bmatrix} 0 \\ 37.2231 \\ 45.628 \\ 51.8268 \\ 58.8182 \\ 67.0839 \end{bmatrix}$$

$$\left(\frac{\text{dcell6}}{\text{dcell8}} \right)^2 = 1.3667$$

Use 600 cells/in2 in recuperator dimension for conservative calculation of CH4, C7H14, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$\text{Numavgrec6c1}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lrec} \cdot 1.1}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}} \quad \text{Numavgrec6c1} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9765 \end{bmatrix}$$

$$\text{Numavgrec6c7}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lrec} \cdot 1.1}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc7T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}} \quad \text{Numavgrec6c7} = \begin{bmatrix} 0 \\ 2.9765 \\ 2.977 \\ 2.9775 \\ 2.9784 \\ 2.9891 \end{bmatrix}$$

$$\text{Numavgrec6co}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lrec} \cdot 1.1}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{SccoT}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dccl6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}} \quad \text{Numavgrec6co} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9766 \end{bmatrix}$$

Once again the entrance effects within the recuperator are negligible

The average (integral) Nusselt numbers at 1-atm show very little contribution of the thermal entry length, i.e. the flow velocities and heat and mass transfer coefficients have values close to those in long channels.

Now determine the maximum possible CH4, C7H14, and CO conversions in a 600 cells per in2 recuperator

$$\text{ych40} = 0.005$$

$$\text{yc7h140} = 0.0005$$

$$\text{yc0} = 0.005$$

Start with maximum concentrations of added pollutants

$$\text{ych4rec6}_{j\text{case}+1} = \text{ych40} \cdot \exp \left(\frac{-4 \cdot \text{Lrec} \cdot 1.1 \cdot \text{Numavgrec6c1}_{j\text{case}+1}}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dccl6}} \right)$$

$$\frac{4 \cdot \text{Lrec} \cdot 1.1 \cdot \text{Numavgrec6c1}_{j\text{case}+1}}{\text{Rerec6}(\text{Grec}_{j\text{case}+1}, \text{Tavg}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Tavg}_{j\text{case}+1}) \cdot \text{dccl6}}$$

65.4083
50.9771
42.7552
35.7764
19.0017

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{ych4rec6} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{ych40} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$5.5932 \cdot 10^{-9}$

$$yc7h14rec6_{jcase+1} = yc7h140 \cdot \exp \left(\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6c7_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot Sc7T(Tavg_{jcase+1}) \cdot dcell6} \right)$$

$$yc7h14rec6 = \begin{bmatrix} 0 \\ 3.5287 \cdot 10^{-12} \\ 2.1834 \cdot 10^{-10} \\ 2.2859 \cdot 10^{-9} \\ 1.6805 \cdot 10^{-8} \\ 2.0597 \cdot 10^{-6} \end{bmatrix} \quad \frac{yc7h14rec6}{yc7h140} = \begin{bmatrix} 0 \\ 7.057 \cdot 10^{-9} \\ 4.367 \cdot 10^{-7} \\ 4.572 \cdot 10^{-6} \\ 3.361 \cdot 10^{-5} \\ 4.119 \cdot 10^{-3} \end{bmatrix} \quad \frac{4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6c7_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot Sc7T(Tavg_{jcase+1}) \cdot dcell6}$$

-18.7692
-14.6441
-12.2956
-10.3007
-5.492

$$ycorec6_{jcase+1} = yco0 \cdot \exp \left(\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6co_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot ScCoT(Tavg_{jcase+1}) \cdot dcell6} \right)$$

$$ycorec6 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1.457 \cdot 10^{-10} \end{bmatrix} \quad \frac{ycorec6}{yco0} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 6.4676 \cdot 10^{-15} \\ 2.914 \cdot 10^{-8} \end{bmatrix} \quad \frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6co_{jcase+1}}{Rerec6(Grec_{jcase+1}, Tavg_{jcase+1}) \cdot ScCoT(Tavg_{jcase+1}) \cdot dcell6}$$

-59.7854
-46.5803
-39.0561
-32.672
-17.3512

With 5000ppm C7H14 in turbine exhaust, exit concentration reaches 20 ppm at the highest power level for conservative 600 cells/in2 calculation. For 800 cells/in2, the exit concentration in this case would reach about 2 ppm. With only 500ppm C7H14 in the inlet, should get <2 ppm in the outlet of the recuperator assuming favorable catalytic rates at the wall. Also this calculation used averaged temperature and flow conditions - will compare below a 1-dimensional (axial) calculation that determines the effect of decreasing temperature on the kinetics and mass transport.

Maximum possible (transport-limited) CO and CH4 conversions in a 7 in. 600-800 cells/in2 recuperator are >99.99%, while cyclohexane conversion is >99.6%. The final CO and C7H14 levels are < 1 ppb and .2 ppm for post turbine concentrations of 1000 and 50 ppm, respectively.

An alternative method of calculating performance uses local Nusselt numbers for heat and mass transfer to determine the wall temperature and combustion rates at the wall. First we define the local Nu function then check conversion assuming fast kinetics and compare with the previous averaged (integrated) Nu formula.

Local Nu(x) taken from Kays & Crawford for hydro & thermal laminar flow entrance with circular channel (modified for square channel by a factor 2.96/3.66:

ncase = 5

$$\text{Numono}(z) := (1 + \exp(-1.09689 - 0.381402 \cdot \ln(z) - 8.287774 \cdot z^{0.5})) \cdot 2.976 \quad \text{Numono}(0.1152163) = 3.112$$

$$\text{zzchar6c7}_{j\text{case}+1} = \frac{\text{Rrec6}(\text{Grec}_{j\text{case}+1}, \text{Trecin}_{j\text{case}+1}) \cdot \text{Sc7T}(\text{Trecin}_{j\text{case}+1}) \cdot \text{dcell6}}{2}$$

$$\frac{\text{Lrec}}{\text{zzchar6c7}_{\text{ncase}}} = 0.9444$$

Case specific

$$\text{zzchar6c1}_{j\text{case}+1} = \frac{\text{Rrec6}(\text{Grec}_{j\text{case}+1}, \text{Trecin}_{j\text{case}+1}) \cdot \text{Sc1T}(\text{Trecin}_{j\text{case}+1}) \cdot \text{dcell6}}{2}$$

$$\frac{\text{Lrec}}{\text{zzchar6c1}_{\text{ncase}}} = 3.2574$$

Case specific

$$\text{nz} := 400$$

$$\text{iz} := 0 \dots \text{nz}$$

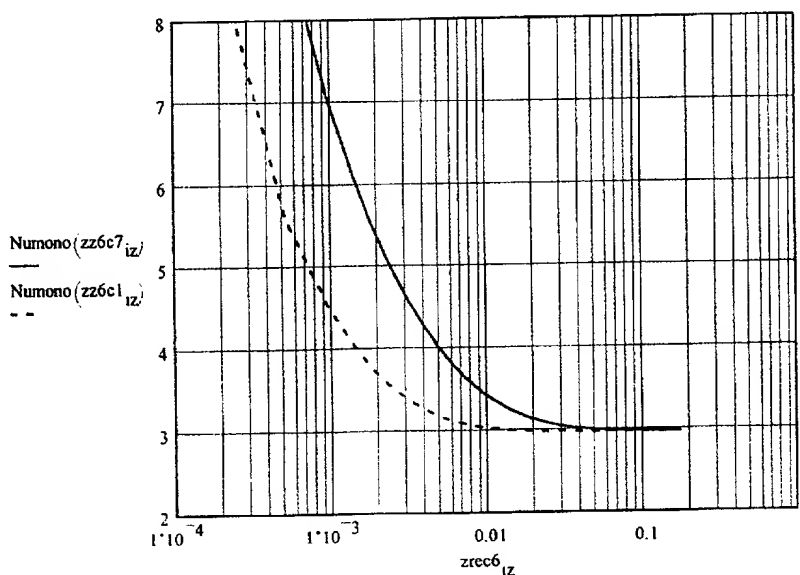
$$\text{Lrec} = 17.78 \cdot \text{cm} \quad \text{dcell6} = 0.0961 \cdot \text{cm}$$

$$\text{zrec6}_{\text{iz}} := \text{iz} \cdot \frac{\text{Lrec}}{\text{nz}} + \text{dwall6}$$

$$\text{zz6c7}_{\text{iz}} = \frac{\text{zrec6}_{\text{iz}}}{\text{zzchar6c7}_{\text{ncase}}} \quad \text{zz6c1}_{\text{iz}} = \frac{\text{zrec6}_{\text{iz}}}{\text{zzchar6c1}_{\text{ncase}}}$$

$$\text{zzchar6c7} = \begin{bmatrix} 0 \\ 4.896 \\ 6.3647 \\ 7.6867 \\ 9.3023 \\ 18.8265 \end{bmatrix} \cdot \text{cm}$$

$$\text{zzchar6c1} = \begin{bmatrix} 0 \\ 1.4244 \\ 1.8518 \\ 2.2364 \\ 2.7064 \\ 5.4583 \end{bmatrix} \cdot \text{cm}$$



Case specific ncase = 5

Case specific ncase = 5

$$kgpb16c7(T, z) = \frac{Dc7h14T(T) \cdot Numono \left(\frac{z}{zzchar6c7_{ncase}} \right)}{dcell6}$$

$$kgpb16c7(Trecin_{ncase}, Lrec) = 13.6159 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kgpb16c1(T, z) = \frac{Dch4T(T) \cdot Numono \left(\frac{z}{zzchar6c1_{ncase}} \right)}{dcell6}$$

$$kgpb16c1(Trecin_{ncase}, Lrec) = 46.9581 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$Trecz_{iz} = Trecin_{ncase} - \frac{Trecin_{ncase} - Trecout_{ncase}}{nz} \cdot iz$$

$$Trecz_{nz} = 630.3722 \cdot \text{K}$$

$$Trecout_{ncase} = 630.3722 \cdot \text{K}$$

Determine maximum conversion of fuels with very fast catalytic combustion rates (zero fuel concentration at the wall)

ncase = 5

$$yzc7h14_0 = yzc7h140$$

$$yzch4_0 = ych40$$

$$yzc7h14_{iz+1} = \left(1 - kgpb16c7(Trecz_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon_{cell6}}{Urec_{ncase}} \cdot \frac{Trecin_{ncase}}{Trecz_{iz}} \right) \cdot yzc7h14_{iz}$$

Case specific

$$yzch4_{iz+1} = \left(1 - kgpb16c1(Trecz_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon_{cell6}}{Urec_{ncase}} \cdot \frac{Trecin_{ncase}}{Trecz_{iz}} \right) \cdot yzch4_{iz}$$

Case specific

$$yzc7h14_{nz} = 3.385 \cdot 10^{-6}$$

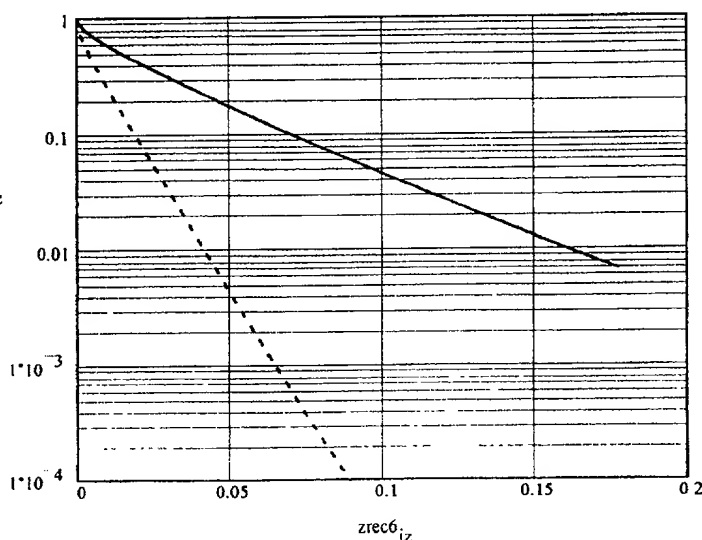
$$yzc7h14_0 = 0.0005$$

$$\frac{yzc7h14_{nz}}{yzc7h14_0} = 6.77 \cdot 10^{-3}$$

$$\frac{yzch4_{nz}}{yzch4_0} = 4.3292 \cdot 10^{-8}$$

$$yzch4_{nz} = 2.1646 \cdot 10^{-10}$$

$$yzch4_0 = 0.005$$



Conversion of C7H14 under case 5 (full power) is 99.3% [vs. 99.6% via averaged integrated formulas] with about 1 inch entry length. Conversion of CH4 (and also CO) is very high (>99.99%) within 3.5 inches.

This result shows that the averaged integrated values for CH4, C7H14, and CO conversions are very good approximations and can be used for different values of fuel and CO concentrations.

Case specific ncase = 5

Add finite rate kinetics for PdO/Al₂O₃ methane combustion catalyst
Begin by defining a few constants and catalyst functions

$$R = 82.076 \cdot K^{-1} \cdot atm \cdot cm^3 \quad atm \cdot cm^3 / mol \cdot K$$

$$R_{cm} = 83143000 \cdot gm \cdot cm^2 \cdot sec^{-2} \cdot K^{-1} \quad TOL = 0.0001$$

Define Catalyst Functions:

$$\eta_{sph}(\phi) = \frac{3}{\phi} \left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi} \right)$$

$$\eta_{fpl}(\phi) = \frac{\tanh(\phi)}{\phi}$$

Catalyst Physical Properties for Pd/Al₂O₃

$$Scat := 85 \cdot m^2 \cdot gm^{-1} \quad \rho_{catpart} = 2.5 \cdot gm \cdot cm^{-3}$$

$$V_{\mu pore} := 0.15 \cdot cm^3 \cdot gm^{-1} \quad d_{pcat} = 0.0002 \cdot cm$$

$$L_{cat} := 0.0020 \cdot cm$$

$$d_{\mu pore} := 6 \cdot \frac{V_{\mu pore}}{Scat} \quad \epsilon_{\mu pore} = 0.375 \quad \tau_{\mu pore} = 3.0$$

$$d_{\mu pore} = 1.0588 \cdot 10^{-6} \cdot cm$$

$$DeffCH4(T) = \frac{\epsilon_{\mu pore}}{\tau_{\mu pore}} \left(\frac{1}{Dch4T(T)} + \frac{3}{d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot MW_0}}} \right)$$

$$d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot Tin}{\pi \cdot MW_0}} = 0.1095 \cdot sec^{-1} \cdot cm^2$$

$$DeffCH4(Tin) = 4.43271 \cdot 10^{-3} \cdot sec^{-1} \cdot cm^2$$

$$Dch4T(Tin) = 1.2343 \cdot sec^{-1} \cdot cm^2$$

$$DeffC7H14(T) = \frac{1}{Dc7h14T(T)} + \frac{3}{d\mu_{pore} \cdot \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot MW_6}}}$$

$$d\mu_{pore} \cdot \frac{\pi}{MW_6} = 0.0829 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$DeffC7H14(Tin) = 3.20528 \cdot 10^{-3} \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$Dc7h14(Tin) = 0.356 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$DmacCH4(T) = \frac{0.4}{2.5} \cdot Dch4T(T)$$

$$DmacCH4(800 \cdot K) = 0.193 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$DmacC7H14(T) = \frac{0.4}{2.5} \cdot Dc7h14T(T)$$

$$DmacC7H14(800 \cdot K) = 0.0556 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$k0T = 1.0 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

Test value for k0T

Microscopic Thiele Modulus for CH4

$$\phi\mu(k, T) = \sqrt{\left[\rho_{catpart} \cdot \left(\frac{R \cdot T}{Pref} \right) \cdot \frac{k}{DeffCH4(T)} \right] \cdot \frac{dpcat}{6}}$$

$$\phi\mu(k0T, Tin) = 0.2042$$

Macroscopic Thiele Modulus for CH4

$$\Phi_{mac}(k, T) = \sqrt{\left[\rho_{catpart} \cdot \left(\frac{R \cdot T}{Pref} \right) \cdot k \right] \cdot \frac{\eta_{sph}(\phi\mu(k, T))}{DmacCH4(T)} \cdot L_{cat}}$$

$$\Phi_{mac}(k0T, Tin) = 1.8333$$

Microscopic Thiele Modulus for C7H14

$$\phi\mu_7(k, T) = \sqrt{\left[\rho_{catpart} \cdot \left(\frac{R \cdot T}{Pref} \right) \cdot \frac{k}{DeffC7H14(T)} \right] \cdot \frac{dpcat}{6}}$$

$$\phi\mu_7(k0T, Tin) = 0.2402$$

Macroscopic Thiele Modulus for C7H14

$$\Phi_{mac7}(k, T) = \sqrt{\left[\rho_{catpart} \cdot \left(\frac{R \cdot T}{Pref} \right) \cdot k \right] \cdot \frac{\eta_{sph}(\phi\mu_7(k, T))}{DmacC7H14(T)} \cdot L_{cat}}$$

$$\Phi_{mac7}(k0T, Tin) = 3.4117$$

$$RatekCH4(k, T) = \eta_{sph}(\phi\mu(k, T)) \cdot \eta_{fp}(\Phi_{mac}(k, T)) \cdot \left[\rho_{catpart} \cdot \left(\frac{R \cdot T}{Pref} \right) \cdot k \right]$$

$$RatekCH4(k0T, Tin) = 85999.4914 \cdot \text{sec}^{-1}$$

$$RatekC7H14(k, T) = \eta_{sph}(\phi\mu_7(k, T)) \cdot \eta_{fp}(\Phi_{mac7}(k, T)) \cdot \left[\rho_{catpart} \cdot \left(\frac{R \cdot T}{Pref} \right) \cdot k \right]$$

$$RatekC7H14(k0T, Tin) = 48479.296 \cdot \text{sec}^{-1}$$

 Defines transport restricted rate constant function given catalyst effective first order rate constant,
 k_0T , methane or cyclohexane concentration, x , and surface temperature, T

PdO Catalyst Rate Constants

$$\text{Erpd0} = 12800 \cdot \text{K} \quad \text{Erpd1} = 4900 \cdot \text{K} \quad \text{Erpd3} = 15000 \cdot \text{K}$$

Region0 - low T PdO to 625K Region1 - Intermediate T Region2 - Flat 909K Region3 -
 ignores inhibition by H₂O and CO₂ 625K to 909K to 1048K decomposition Pd metal

$$\text{Apd0} := 2.4 \cdot 10^3 \cdot 200 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1} \quad \text{Apd1} = \text{Apd0} \cdot \exp\left(-\frac{\text{Erpd0}}{625 \cdot \text{K}} + \frac{\text{Erpd1}}{625 \cdot \text{K}}\right)$$

$$\text{Apd2} := \text{Apd1} \cdot \exp\left(-\frac{\text{Erpd1}}{909.1 \cdot \text{K}}\right) \quad \text{Apd3} = \text{Apd2} \cdot \exp\left(-\frac{\text{Erpd3}}{1048.1 \cdot \text{K}}\right)$$

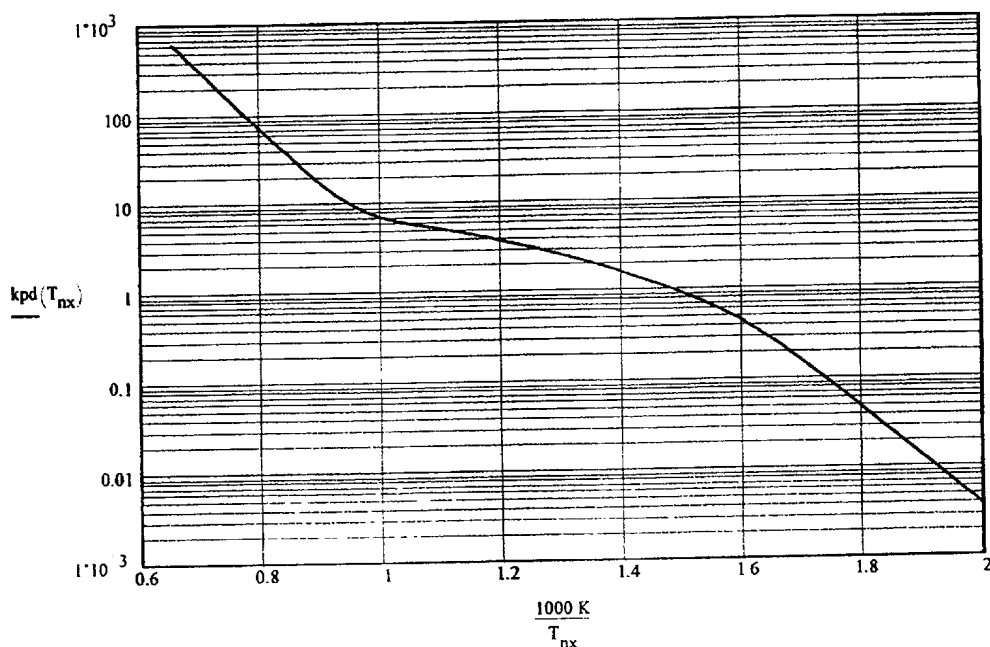
Interpolation formula for the four PdO+Pd rate constants

$$kpd(T) := \left[\text{Apd3}^2 \cdot \exp\left(-\frac{2 \cdot \text{Erpd3}}{T}\right) + \frac{1}{\left(\text{Apd2}^{-2} + \text{Apd1}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd1}}{T}\right) + \text{Apd0}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd0}}{T}\right) \right)} \right]^{0.5}$$

$$nx := 0, 1 \dots 41$$

$$T_{nx} = 500 \cdot \text{K} + nx \cdot 25 \cdot \text{K}$$

CATALYTIC RATE CONSTANT vs TEMPERATURE (mol/atmCH₄/s/gcat)

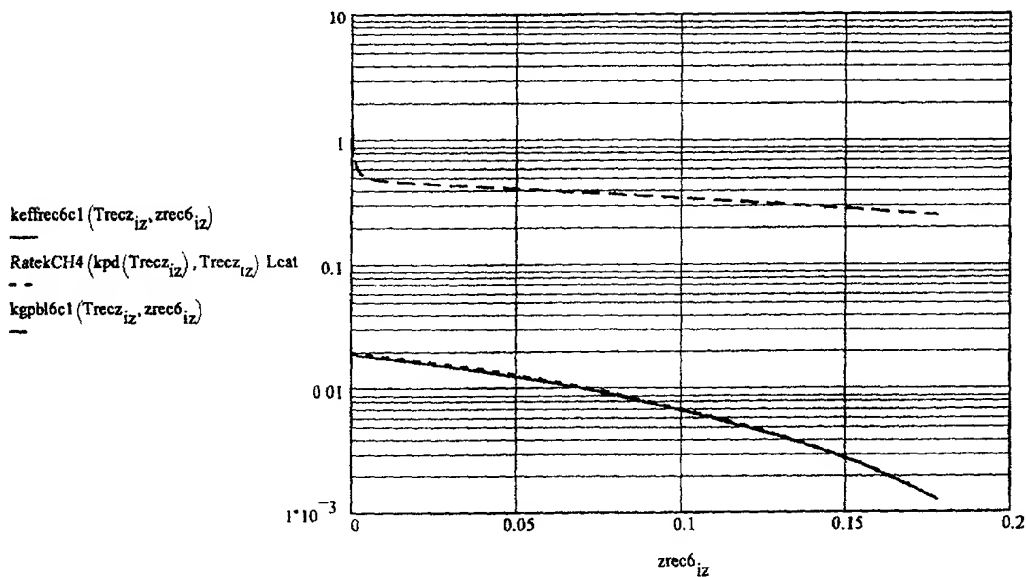


$$\text{keffrec6c1}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekCH4}(\text{kpd}(T), T) \cdot \text{Lcat}} \right) + \frac{1}{\text{kgpbl6c1}(T, z)}} \quad \text{kgpbl6c1}\left(\text{Tavg}_{\text{nCase}}, \frac{\text{Lrec}}{2}\right) = 35.3023 \cdot \text{sec}^{-1} \cdot \text{cm}$$

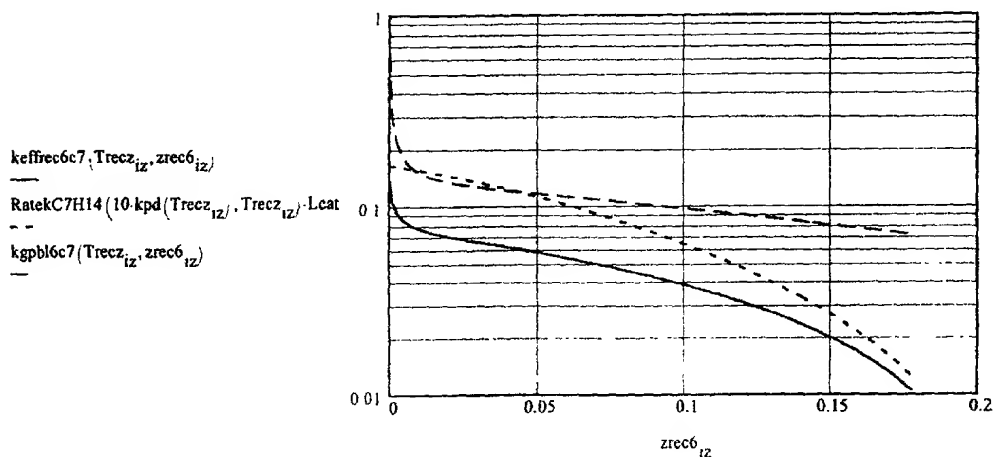
$$\text{keffrec6c1}\left(\text{Tavg}_{\text{nCase}}, \frac{\text{Lrec}}{2}\right) = 0.7922 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekCH4}\left(\text{kpd}(\text{Tavg}_{\text{nCase}}), \text{Tavg}_{\text{nCase}}\right) \cdot \text{Lcat} = 0.8104 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekC7H14}(10 \cdot \text{kpd}(T), T) \cdot \text{Lcat}} \right) + \frac{1}{\text{kgpbl6c7}(T, z)}} \quad \text{kgpbl6c7}\left(\text{Tavg}_{\text{nCase}}, \frac{\text{Lrec}}{2}\right) = 10.1756 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}\left(\text{Tavg}_{\text{nCase}}, \frac{\text{Lrec}}{2}\right) = 4.2778 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekC7H14}\left(10 \cdot \text{kpd}(\text{Tavg}_{\text{nCase}}), \text{Tavg}_{\text{nCase}}\right) \cdot \text{Lcat} = 7.3807 \cdot \text{sec}^{-1} \cdot \text{cm}$$



Case specific ncase = 5



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $ncase = 5$

$$Trecz_{iz} = Trecin_{ncase} - \frac{Trecin_{ncase} - Trecout_{ncase}}{nz} \cdot iz$$

$$Trecz_{nz} = 630.3722 \cdot K$$

$$Trecout_{ncase} = 630.3722 \cdot K$$

$$yzkc7h14_0 = yc7h140$$

$$yzkch4_0 = ych40$$

$$yzkc7h14_{iz+1} = \left(1 - keffrec6c7(Trecz_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon_{cell6}}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}} \right) \cdot yzkc7h14_{iz}$$

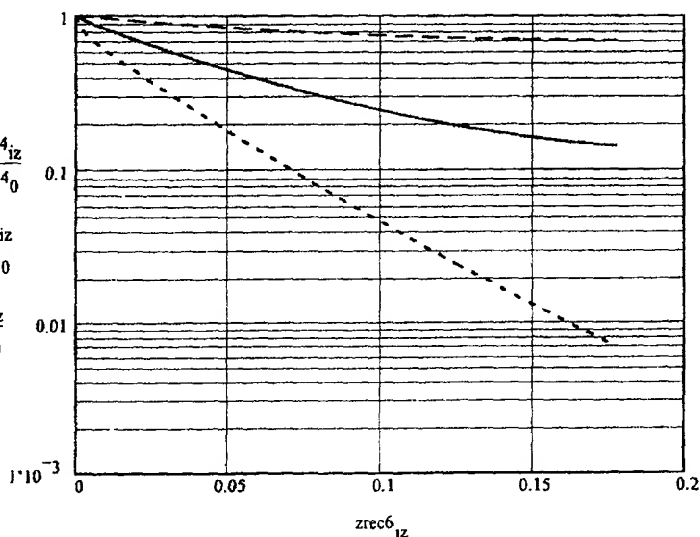
Case specific

$ncase = 5$

$$yzkch4_{iz+1} = \left(1 - keffrec6cl(Trecz_{iz}, zrec6_{iz}) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon_{cell6}}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}} \right) \cdot yzkch4_{iz}$$

Case specific

$$\begin{aligned} yzkc7h14_{nz} &= 7.036 \cdot 10^{-5} & yzkc7h14_0 &= 0.0005 & \frac{yzkc7h14_{nz}}{yzkc7h14_0} &= 1.407 \cdot 10^{-1} & \frac{yzkch4_{nz}}{yzkch4_0} &= 0.6838 \\ yzkch4_{nz} &= 0.0034 & yzkch4_0 &= 0.005 \end{aligned}$$



Case specific $ncase = 5$

Conversion of C7H14 under case 5 (full power) is 99.4% [vs. 99.3% for the maximum BL transport-limited conversion] with gradually decreasing (rate limited) conversion. Conversion of CH4 is very poor (35%). CO conversion is probably very high given higher catalytic and transport rates than with C7H14.

This result shows that the specific rates of catalytic oxidation of all added components needs to be measured as applied to a recuperator. The use of a recuperator for emission control would appear to be greatly enhanced with higher exhaust (recuperator) temperatures.

In the following section, the conversion of C7H14, CH4 and CO is considered for various honeycomb monoliths

$$Thc_{jcase+1} = Trecin_{jcase+1}$$

$$\rho_{mixhc}_{jcase+1} = \rho_{mixrec}(Trecin_{jcase+1})$$

$$Ghc2_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell2}$$

$$Ghc4_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell4}$$

$$Ghc6_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell6}$$

$$Uhc2 = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc4 = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc6 = \begin{bmatrix} 0 \\ 3.1706 \\ 4.1218 \\ 4.9779 \\ 6.0242 \\ 10.4051 \end{bmatrix} \cdot m \cdot sec^{-1}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$Rehc2_{jcase+1} = \frac{Ghc2_{jcase+1} \cdot dcell2}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc4_{jcase+1} = \frac{Ghc4_{jcase+1} \cdot dcell4}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc6_{jcase+1} = \frac{Ghc6_{jcase+1} \cdot dcell6}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc2 = \begin{bmatrix} 0 \\ 43.776 \\ 56.9088 \\ 68.7283 \\ 83.1744 \\ 167.4548 \end{bmatrix}$$

$$Rehc4 = \begin{bmatrix} 0 \\ 31.7427 \\ 41.2655 \\ 49.836 \\ 60.3111 \\ 121.4242 \end{bmatrix}$$

$$Rehc6 = \begin{bmatrix} 0 \\ 25.7355 \\ 33.4562 \\ 40.4048 \\ 48.8975 \\ 98.4453 \end{bmatrix}$$

$$cfrichc2(j,z) = \frac{14.227}{Rehc2_j} \left[1 + 0.046263 \cdot \left(Rehc2_j \cdot \frac{dcell2}{z} \right) \right]^{0.45363}$$

$$cfrichc4(j,z) = \frac{14.227}{Rehc4_j} \left[1 + 0.046263 \cdot \left(Rehc4_j \cdot \frac{dcell4}{z} \right) \right]^{0.45363}$$

Average coefficients of friction
for smooth square channels

$$cfrichc6(j,z) = \frac{14.227}{Rehc6_j} \left[1 + 0.046263 \cdot \left(Rehc6_j \cdot \frac{dcell6}{z} \right) \right]^{0.45363}$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta Phc2_{jcase+1} = 4 \cdot cfrichc2(jcase+1, Lhc) \cdot \frac{Uhc2_{jcase+1}^2}{2} \cdot \rho_{mixhc_{jcase+1}} \cdot \frac{Lhc}{dcell2}$$

$$\Delta Phc4_{jcase+1} = 4 \cdot cfrichc4(jcase+1, Lhc) \cdot \frac{Uhc4_{jcase+1}^2}{2} \cdot \rho_{mixhc_{jcase+1}} \cdot \frac{Lhc}{dcell4}$$

$$\Delta Phc6_{jcase+1} = 4 \cdot cfrichc6(jcase+1, Lhc) \cdot \frac{Uhc6_{jcase+1}^2}{2} \cdot \rho_{mixhc_{jcase+1}} \cdot \frac{Lhc}{dcell6}$$

$$\frac{\Delta Phc2}{Phc} = \begin{bmatrix} 0 \\ 0.0013 \\ 0.0017 \\ 0.002 \\ 0.0024 \\ 0.0041 \end{bmatrix}$$

$$\frac{\Delta Phc4}{Phc} = \begin{bmatrix} 0 \\ 0.0028 \\ 0.0036 \\ 0.0044 \\ 0.0053 \\ 0.0088 \end{bmatrix}$$

$$\frac{\Delta Phc6}{Phc} = \begin{bmatrix} 0 \\ 0.004 \\ 0.0053 \\ 0.0064 \\ 0.0077 \\ 0.0127 \end{bmatrix}$$

$$\Delta Phcmax_P = \begin{bmatrix} 0 \\ 0.003 \\ 0.004 \\ 0.005 \\ 0.006 \\ 0.011 \end{bmatrix}$$

Chose 400 cells per in2
honeycombs via estimated ΔP

Use 400 cells/in2 in honeycomb monolith for calculation of CH4, C7H14, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$Numavghc4c1_{jcase+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Rehc4_{jcase+1} \cdot Sc1T(Thc_{jcase+1}) \cdot dcell4} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$Numavghc4c1 = \begin{bmatrix} 0 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9762 \\ 2.9774 \end{bmatrix}$$

$$Numavghc4co_{jcase+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Rehc4_{jcase+1} \cdot ScocT(Thc_{jcase+1}) \cdot dcell4} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$Numavghc4co = \begin{bmatrix} 0 \\ 2.976 \\ 2.9761 \\ 2.9762 \\ 2.9763 \\ 2.9778 \end{bmatrix}$$

$$\text{Numavghc4c7}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lhc}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{Sc7T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{Numavghc4c7} = \begin{bmatrix} 0 \\ 2.977 \\ 2.9781 \\ 2.9795 \\ 2.9817 \\ 3.0123 \end{bmatrix}$$

Once again the entrance effects within monoliths are generally small

Now determine the maximum possible CH₄, C₇H₁₄, and CO conversions in a 400 cells per in² monolith

$$\text{ych40} = 0.005$$

$$\text{yc7h140} = 0.0005$$

$$\text{yco0} = 0.005$$

$$\text{ych4hc4}_{j\text{case}+1} = \text{ych40} \cdot \exp \left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4c1}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}} \right)$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4c1}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}}$$

-48.7678
-37.5142
-31.0633
-25.6688
-12.7326

$$\frac{\text{ych4hc4}}{\text{ych40}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3.2315 \cdot 10^{-14} \\ 7.1151 \cdot 10^{-12} \\ 2.9532 \cdot 10^{-6} \end{bmatrix}$$

$$\text{ycohc4}_{j\text{case}+1} = \text{yco0} \cdot \exp \left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4co}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{SccoT}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}} \right)$$

$$\frac{\text{ycohc4}}{\text{yco0}} = \begin{bmatrix} 0 \\ 0 \\ 1.4726 \cdot 10^{-15} \\ 5.2301 \cdot 10^{-13} \\ 7.0997 \cdot 10^{-11} \\ 9.1398 \cdot 10^{-6} \end{bmatrix}$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc4co}_{j\text{case}+1}}{\text{Rehc4}_{j\text{case}+1} \cdot \text{SccoT}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell4}}$$

-44.3966
-34.1518
-28.2792
-23.3684
-11.6029

$$yc7h14hc4_{jcase+1} = yc7h140 \cdot \exp\left(\frac{4 \cdot Lhc \cdot Numavghc4c7_{jcase+1}}{Rehc4_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell4}\right)$$

$$\frac{4 \cdot Lhc \cdot Numavghc4c7_{jcase+1}}{Rehc4_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell4}$$

-14.1935
-10.9219
9.0478
-7.482
-3.7348

$$\frac{yc7h14hc4}{yc7h140} = \begin{bmatrix} 0 \\ 6.8527 \cdot 10^{-7} \\ 1.8058 \cdot 10^{-5} \\ 0.0001 \\ 0.0006 \\ 0.0239 \end{bmatrix}$$

Only for C7H14 and only in case 5 (maximum power) does the BL transport-only calculated conversion (97.6%) fall below 99.9% with a 400 cells/in² monolith. With 50 ppm C7H14 in the exhaust in this case, the exit concentration would be 1.2 ppm.

For the final analysis, consider the finite catalytic conversion of C7H14 and CH4 in a monolith: mcase = 5

$$zzcharhc4c7_{jcase+1} = \frac{Rehc4_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell4}{2}$$

$$\frac{Lhc}{zzcharhc4c7_{mcase}} = 0.6199$$

$$zzcharhc4c1_{jcase+1} = \frac{Rehc4_{jcase+1} \cdot Sc1T(Trecin_{jcase+1}) \cdot dcell4}{2}$$

$$\frac{Lhc}{zzcharhc4c1_{mcase}} = 2.1382$$

$$nz = 400$$

$$Lhc = 10.16 \text{ cm} \quad dcell4 = 0.1168 \text{ cm}$$

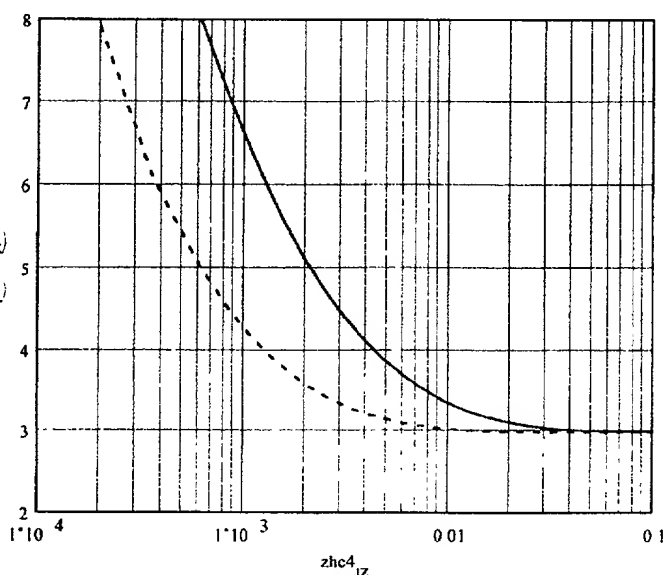
$$zhc4_{iz} = iz \cdot \frac{Lhc}{nz} + dwall4$$

$$zzhc4c7_{iz} = \frac{zhc4_{iz}}{zzcharhc4c7_{mcase}}$$

$$zzhc4c1_{iz} = \frac{zhc4_{iz}}{zzcharhc4c1_{mcase}}$$

$$zzcharhc4c7 = \begin{bmatrix} 0 \\ 4.2621 \\ 5.5407 \\ 6.6914 \\ 8.0979 \\ 16.389 \end{bmatrix} \text{ cm}$$

Numono(zzhc4c7_{iz})
 Numono(zzhc4c1_{iz})
 --



Case specific mcase = 5

$$kgpblhc4c7(T, z) = \frac{Dc7h14T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc4c7_{mcase}}\right)}{dcell4}$$

$$kgpblhc4c7(Thc_{mcase}, Lhc) = 11.2014 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kgpblhc4c1(T, z) = \frac{Dch4T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc4c1_{mcase}}\right)}{dcell4}$$

$$kgpblhc4c1(Thc_{mcase}, Lhc) = 38.6127 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc4c1(T, z) = \frac{1}{\left(\frac{1}{\text{RatekCH4}(kpd(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc4c1(T, z)}}$$

$$kgpblhc4c1\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 38.615 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc4c1\left(Thc_{mcase}, \frac{Lrec}{2}\right) = 1.8533 \cdot \text{sec}^{-1} \cdot \text{cm}$$

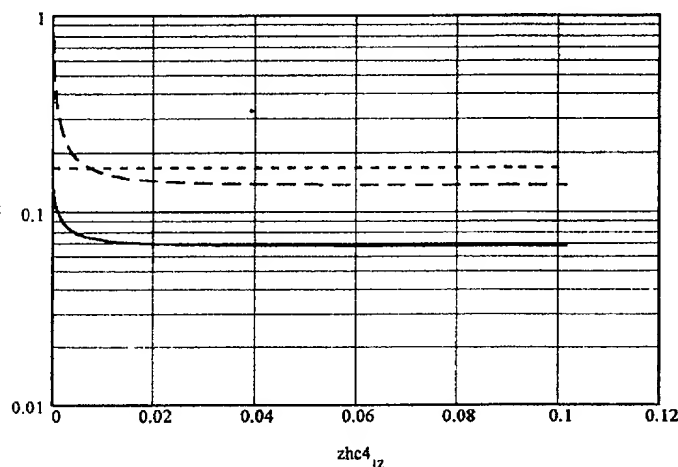
$$\text{RatekCH4}(kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 1.9467 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc4c7(T, z) = \frac{1}{\left(\frac{1}{\text{RatekC7H14}(10 \cdot kpd(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc4c7(T, z)}}$$

$$kgpblhc4c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 11.2528 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc4c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 6.7062 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{RatekC7H14}(10 \cdot kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 16.5977 \cdot \text{sec}^{-1} \cdot \text{cm}$$



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $m_{case} = 5$

$$yzkhc4c7h14_0 = yc7h140$$

$$yzkhc4ch4_0 = ych40$$

$$yzkhc4c7h14_{iz+1} = \left(1 - keffhc4c7(T_{hc_{mcase}}, zhc4_{iz}) \cdot \frac{L_{hc}}{nz} \cdot \frac{4}{dcell4} \cdot \frac{\epsilon_{cell4}}{U_{hc4_{mcase}}} \right) \cdot yzkhc4c7h14_{iz}$$

$$yzkhc4ch4_{iz+1} = \left(1 - keffhc4c1(T_{hc_{mcase}}, zhc4_{iz}) \cdot \frac{L_{hc}}{nz} \cdot \frac{4}{dcell4} \cdot \frac{\epsilon_{cell4}}{U_{hc4_{mcase}}} \right) \cdot yzkhc4ch4_{iz}$$

$$T_{hc} = \begin{bmatrix} 0 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 916.4833 \end{bmatrix} \cdot K$$

Case specific

$m_{case} = 5$

$$yzkhc4c7h14_{nz} = 7.281 \cdot 10^{-5}$$

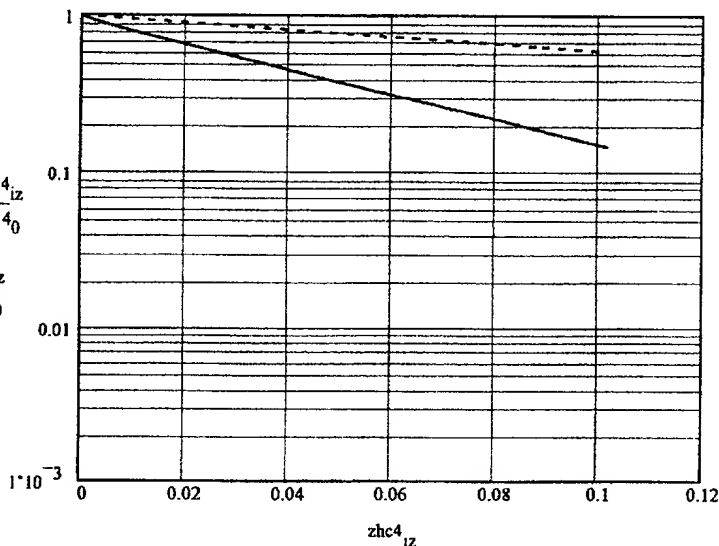
$$yzkhc4c7h14_0 = 0.0005$$

$$yzkhc4ch4_{nz} = 0.003$$

$$yzkhc4ch4_0 = 0.005$$

$$\frac{yzkhc4c7h14_{nz}}{yzkhc4c7h14_0} = 1.456 \cdot 10^{-1}$$

$$\frac{yzkhc4ch4_{nz}}{yzkhc4ch4_0} = 0.5959$$



Case specific $m_{case} = 5$

Conversion of C7H14 under case 5 (full power) is 99.4% [vs. 99.6% via averaged integrated formulas] with about 1-inch entry length. Conversion of CH4 (and also CO) is very high (>99.99%) within about 3.5-inch.

This result shows that the averaged integrated values for CH4, C7H14, and CO conversions are very good approximations and can be used for different values of fuel and CO concentrations.

 Defines transport restricted rate constant function given catalyst effective first order rate constant,
 k_0T , methane or cyclohexane concentration, x , and surface temperature, T

PdO Catalyst Rate Constants

$$Erpd0 = 12800 \cdot K \quad Erpd1 = 4900 \cdot K \quad Erpd3 = 15000 \cdot K$$

Region0 - low T PdO to 625K
 ignores inhibition by H₂O and CO₂

Region1 - Intermediate T
 625K to 909K

Region2 - Flat 909K
 to 1048K decomposition

Region3 -
 Pd metal

$$Apd0 = 2.4 \cdot 10^3 \cdot 200 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

$$Apd1 = Apd0 \cdot \exp\left(-\frac{Erpd0}{625 \cdot K} + \frac{Erpd1}{625 \cdot K}\right)$$

$$Apd2 = Apd1 \cdot \exp\left(-\frac{Erpd1}{909.1 \cdot K}\right)$$

Interpolation formula for the four PdO+Pd rate constants

$$Apd3 = Apd2 \cdot \exp\left(\frac{Erpd3}{1048.1 \cdot K}\right)$$

$$kpd(T) = \left[Apd3^2 \cdot \exp\left(-\frac{2 \cdot Erpd3}{T}\right) + \frac{1}{\left(Apd2^{-2} + Apd1^{-2} \cdot \exp\left(\frac{2 \cdot Erpd1}{T}\right) + Apd0^{-2} \cdot \exp\left(\frac{2 \cdot Erpd0}{T}\right) \right)} \right]^{0.5}$$

Add expression for Pt(.5%)Pd(3.0%) catalyst with C₃H₈ here, use x2 for estimated rate constant with C₇H₁₄:

Rate constant via crushed powder results for C₃H₈

$$ktpdC3(T) = 6.9 \cdot 10^4 \cdot \exp\left(-\frac{10760 \cdot K}{T}\right) \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

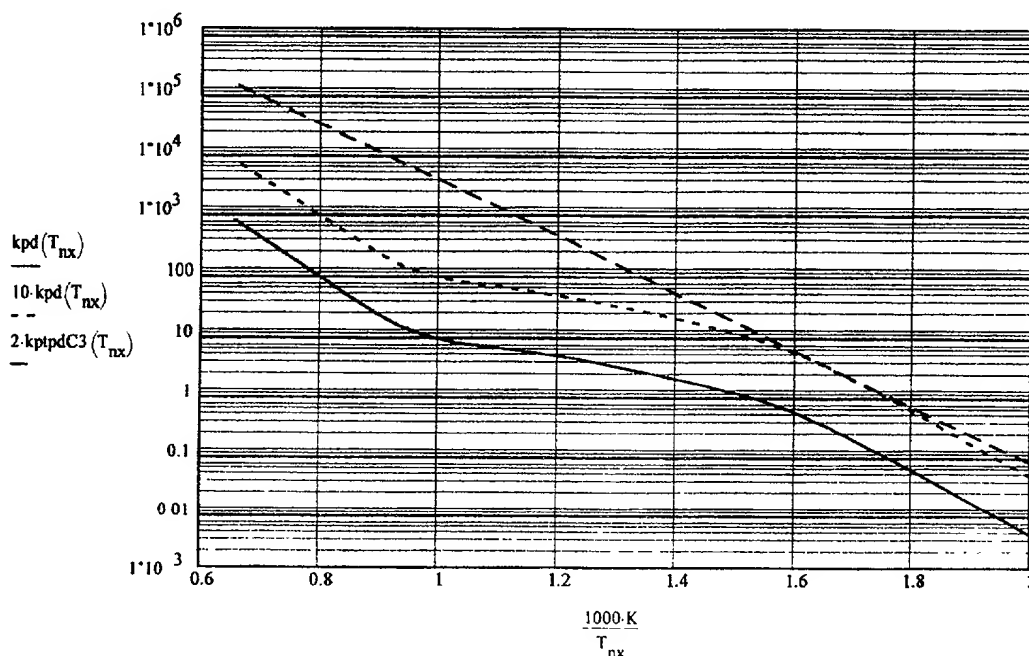
$$10 \cdot kpd(900 \cdot K) = 49.2392 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$2 \cdot ktpdC3(900 \cdot K) = 886.4358 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$nx = 0, 1 \dots 41$$

$$T_{nx} = 500 \cdot K + nx \cdot 25 \cdot K$$

CATALYTIC RATE CONSTANT vs TEMPERATURE (mol/atmCHx/s/gcat)

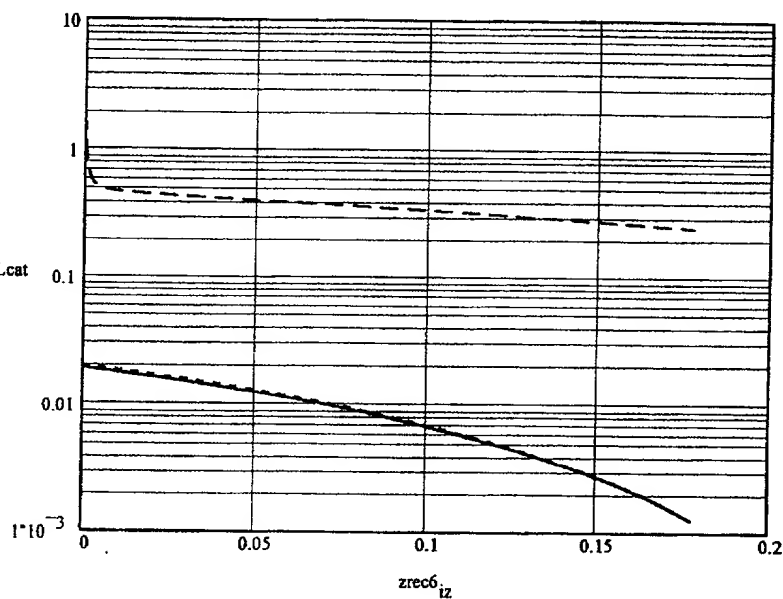


$$\text{keffrec6c1}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekCH4}(\text{kpd}(T), T) \cdot \text{Lcat}} \right) + \frac{1}{\text{kgpbl6c1}(T, z)}} \quad \text{kgpbl6c1}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 35.3023 \cdot \text{sec}^{-1} \cdot \text{cm}$$

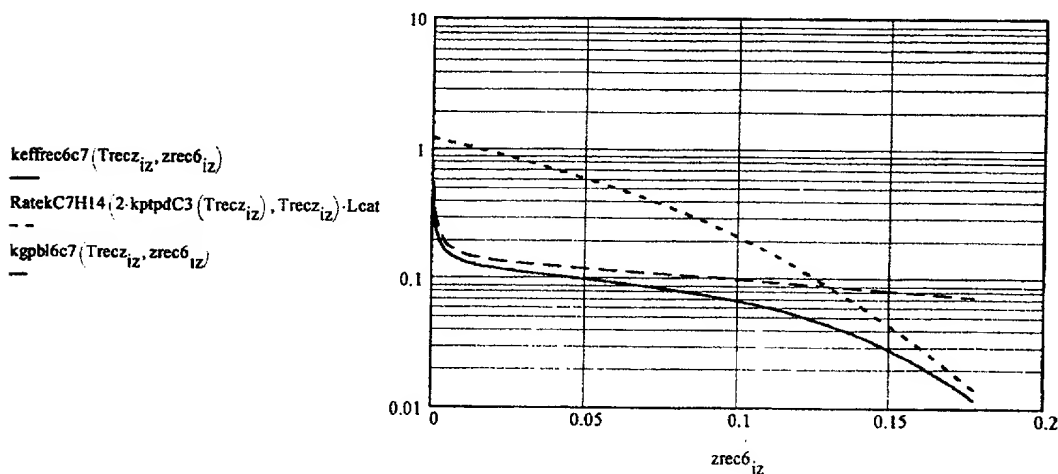
$$\text{keffrec6c1}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 0.7922 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekCH4}(\text{kpd}(\text{Tavg}_{\text{ncase}}), \text{Tavg}_{\text{ncase}}) \cdot \text{Lcat} = 0.8104 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}(T, z) = \frac{1}{\left(\frac{1}{\text{RatekC7H14}(2 \cdot \text{ktpdC3}(T), T) \cdot \text{Lcat}} \right) + \frac{1}{\text{kgpbl6c7}(T, z)}} \quad \text{kgpbl6c7}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 10.1756 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{keffrec6c7}\left(\text{Tavg}_{\text{ncase}}, \frac{\text{Lrec}}{2}\right) = 7.4067 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekC7H14}(2 \cdot \text{ktpdC3}(\text{Tavg}_{\text{ncase}}), \text{Tavg}_{\text{ncase}}) \cdot \text{Lcat} = 27.2196 \cdot \text{sec}^{-1} \cdot \text{cm}$$



Case specific $\text{ncase} = 5$



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

$$\text{Trecz}_{iz} = \text{Trecin}_{ncase} - \frac{\text{Trecin}_{ncase} - \text{Trecout}_{ncase}}{nz} \cdot iz$$

Case specific $ncase = 5$

$$\text{Trecz}_{nz} = 630.3722 \cdot K \quad \text{Trecout}_{ncase} = 630.3722 \cdot K$$

$$\text{yzkc7h14}_0 = \text{yc7h140} \quad \text{yzkch4}_0 = \text{ych40}$$

$$\text{yzkc7h14}_{iz+1} = \left(1 - \text{keffrec6c7}(\text{Trecz}_{iz}, \text{zrec6}_{iz}) \cdot \frac{\text{Lrec}}{nz} \cdot 1.1 \cdot \frac{4}{\text{dcell6}} \cdot \frac{\text{ecell6}}{\text{Urec}_{ncase}} \cdot \frac{\text{Trecin}_5}{\text{Trecz}_{iz}} \right) \cdot \text{yzkc7h14}_{iz}$$

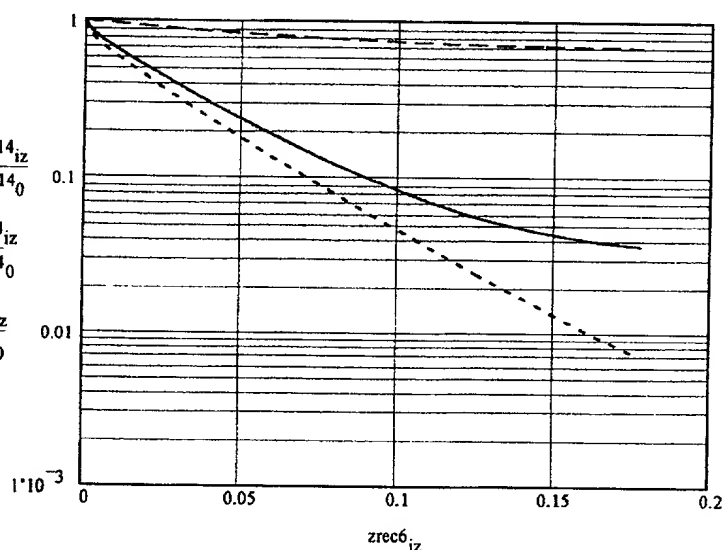
Case specific

$ncase = 5$

$$\text{yzkch4}_{iz+1} = \left(1 - \text{keffrec6c1}(\text{Trecz}_{iz}, \text{zrec6}_{iz}) \cdot \frac{\text{Lrec}}{nz} \cdot 1.1 \cdot \frac{4}{\text{dcell6}} \cdot \frac{\text{ecell6}}{\text{Urec}_{ncase}} \cdot \frac{\text{Trecin}_5}{\text{Trecz}_{iz}} \right) \cdot \text{yzkch4}_{iz}$$

Case specific

$$\begin{aligned} \text{yzkc7h14}_{nz} &= 1.802 \cdot 10^{-5} & \text{yzkc7h14}_0 &= 0.0005 & \frac{\text{yzkc7h14}_{nz}}{\text{yzkc7h14}_0} &= 3.603 \cdot 10^{-2} & \frac{\text{yzkch4}_{nz}}{\text{yzkch4}_0} &= 0.6838 \\ \text{yzkch4}_{nz} &= 0.0034 & \text{yzkch4}_0 &= 0.005 \end{aligned}$$



Case specific $ncase = 5$

Conversion of C7H14 under case 5 (full power) is 97.4% with estimated catalytic rates and transport limitations [vs. 99.6% for the maximum BL transport-limited conversion]. Conversion of CH4 is very poor (32%). CO conversion is probably very high given higher catalytic and transport rates than with C7H14.

This result shows that the specific rates of catalytic oxidation of all added components needs to be measured as applied to a recuperator. The use of a recuperator for emission control would appear to be greatly enhanced with higher exhaust (recuperator) temperatures.

In the following section, the conversion of C7H14, CH4 and CO is considered for various honeycomb monoliths

$$Thc_{jcase+1} = Trecin_{jcase+1} \quad \rho_{mixhc}_{jcase+1} = \rho_{mixrec}(Trecin_{jcase+1})$$

$$Ghc2_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell2} \quad Ghc4_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell4} \quad Ghc6_{jcase+1} = \frac{mf_{jcase+1}}{Shc \cdot dcell6}$$

$$Uhc2 = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc4 = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot m \cdot sec^{-1}$$

$$Uhc6 = \begin{bmatrix} 0 \\ 3.1706 \\ 4.1218 \\ 4.9779 \\ 6.0242 \\ 10.4051 \end{bmatrix} \cdot m \cdot sec^{-1}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$Rehc2_{jcase+1} = \frac{Ghc2_{jcase+1} \cdot dcell2}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc4_{jcase+1} = \frac{Ghc4_{jcase+1} \cdot dcell4}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc6_{jcase+1} = \frac{Ghc6_{jcase+1} \cdot dcell6}{\mu_{mixT}(Thc_{jcase+1})}$$

$$Rehc2 = \begin{bmatrix} 0 \\ 43.776 \\ 56.9088 \\ 68.7283 \\ 83.1744 \\ 167.4548 \end{bmatrix}$$

$$Rehc4 = \begin{bmatrix} 0 \\ 31.7427 \\ 41.2655 \\ 49.836 \\ 60.3111 \\ 121.4242 \end{bmatrix}$$

$$Rehc6 = \begin{bmatrix} 0 \\ 25.7355 \\ 33.4562 \\ 40.4048 \\ 48.8975 \\ 98.4453 \end{bmatrix}$$

$$cfrihc2(j,z) = \frac{14.227}{Rehc2_j} \left[1 + 0.046263 \cdot \left(Rehc2_j \cdot \frac{dcell2}{z} \right)^{0.45363} \right]$$

$$cfrihc4(j,z) = \frac{14.227}{Rehc4_j} \left[1 + 0.046263 \cdot \left(Rehc4_j \cdot \frac{dcell4}{z} \right)^{0.45363} \right]$$

Average coefficients of friction
for smooth square channels

$$cfrihc6(j,z) = \frac{14.227}{Rehc6_j} \left[1 + 0.046263 \cdot \left(Rehc6_j \cdot \frac{dcell6}{z} \right)^{0.45363} \right]$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta P_{hc2, j_{case}+1} = 4 \cdot c_{fric}hc2(j_{case}+1, L_{hc}) \cdot \frac{U_{hc2, j_{case}+1}^2}{2} \cdot \rho_{mix}hc_{j_{case}+1} \cdot \frac{L_{hc}}{d_{cell2}}$$

$$\Delta P_{hc4, j_{case}+1} = 4 \cdot c_{fric}hc4(j_{case}+1, L_{hc}) \cdot \frac{U_{hc4, j_{case}+1}^2}{2} \cdot \rho_{mix}hc_{j_{case}+1} \cdot \frac{L_{hc}}{d_{cell4}}$$

$$\Delta P_{hc6, j_{case}+1} = 4 \cdot c_{fric}hc6(j_{case}+1, L_{hc}) \cdot \frac{U_{hc6, j_{case}+1}^2}{2} \cdot \rho_{mix}hc_{j_{case}+1} \cdot \frac{L_{hc}}{d_{cell6}}$$

$$\frac{\Delta P_{hc2}}{P_{hc}} = \begin{bmatrix} 0 \\ 0.0013 \\ 0.0017 \\ 0.002 \\ 0.0024 \\ 0.0041 \end{bmatrix} \quad \frac{\Delta P_{hc4}}{P_{hc}} = \begin{bmatrix} 0 \\ 0.0028 \\ 0.0036 \\ 0.0044 \\ 0.0053 \\ 0.0088 \end{bmatrix} \quad \frac{\Delta P_{hc6}}{P_{hc}} = \begin{bmatrix} 0 \\ 0.004 \\ 0.0053 \\ 0.0064 \\ 0.0077 \\ 0.0127 \end{bmatrix} \quad \frac{3.5 \cdot \Delta P_{hc6}}{4 \cdot P_{hc}} = \begin{bmatrix} 0 \\ 0.0035 \\ 0.0046 \\ 0.0056 \\ 0.0068 \\ 0.0111 \end{bmatrix} \quad \Delta P_{hcmax_P} = \begin{bmatrix} 0 \\ 0.003 \\ 0.004 \\ 0.005 \\ 0.006 \\ 0.011 \end{bmatrix}$$

Chose 600 cells per in2 honeycombs but
reduce length to 3.5in via estimated ΔP

$$L_{hc} = 3.5 \cdot \text{in}$$

Use 600 cells/in2 in honeycomb monolith for calculation of CH4, C7H14, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$\text{Numavghc6cl}_{j_{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot L_{hc}}{\text{Rehc6}_{j_{case}+1} \cdot \text{ScIT}(\text{Thc}_{j_{case}+1}) \cdot d_{cell6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Numavghc6cl} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9767 \end{bmatrix}$$

$$\text{Numavghc6co}_{j_{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot L_{hc}}{\text{Rehc6}_{j_{case}+1} \cdot \text{ScCoT}(\text{Thc}_{j_{case}+1}) \cdot d_{cell6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Numavghc6co} = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9769 \end{bmatrix}$$

$$\text{Numavghc6c7}_{j\text{case}+1} = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot \text{Lhc}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}} \right)^{\frac{1}{3}} \right]^{\frac{8}{3}}$$

$$\text{Numavghc6c7} = \begin{bmatrix} 0 \\ 2.9765 \\ 2.977 \\ 2.9777 \\ 2.9788 \\ 2.994 \end{bmatrix}$$

Once again the entrance effects within monoliths are generally small

Now determine the maximum possible CH₄, C₇H₁₄, and CO conversions in a 600 cells per in² monolith

$$\text{ych40} := 0.005$$

$$\text{yc7h140} := 0.0005$$

$$\text{yco0} := 0.005$$

$$\text{ych4hc6}_{j\text{case}+1} = \text{ych40} \cdot \exp \left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6c1}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}} \right)$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6c1}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{Sc1T}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}}$$

-64.0074
-49.2367
-40.7696
-33.689
-16.7076

$$\frac{\text{ych4hc6}}{\text{ych40}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 2.339 \cdot 10^{-15} \\ 5.5463 \cdot 10^{-8} \end{bmatrix}$$

$$\text{ycohc6}_{j\text{case}+1} = \text{yco0} \cdot \exp \left(\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6co}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{SccoT}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}} \right)$$

$$\frac{\text{ycohc6}}{\text{yco0}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 4.7906 \cdot 10^{-14} \\ 2.445 \cdot 10^{-7} \end{bmatrix}$$

$$\frac{-4 \cdot \text{Lhc} \cdot \text{Numavghc6co}_{j\text{case}+1}}{\text{Rehc6}_{j\text{case}+1} \cdot \text{SccoT}(\text{Thc}_{j\text{case}+1}) \cdot \text{dcell6}}$$

-58.27
-44.8234
-37.1153
-30.6695
-15.2241

FORCED CONVECTION

$$yc7h14hc6_{jcase+1} = yc7h140 \cdot \exp\left(\frac{-3.5 \cdot Lhc \cdot Numavghc6c7_{jcase+1}}{Rehc6_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell6}\right)$$

$$\frac{-3.5 \cdot Lhc \cdot Numavghc6c7_{jcase+1}}{Rehc6_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell6}$$

-16.2974
-12.5386
-10.3846
-8.5841
-4.2631

$$\frac{yc7h14hc6}{yc7h140} = \begin{bmatrix} 0 \\ 8.3588 \cdot 10^{-8} \\ 3.5856 \cdot 10^{-6} \\ 3.0905 \cdot 10^{-5} \\ 0.0002 \\ 0.0141 \end{bmatrix}$$

Only for C7H14 and only in case 5 (maximum power) does the BL transport-only calculated conversion (98.6%) fall below 99.9% with a 600 cells/in² monolith. With 50 ppm C7H14 in the exhaust in this case, the exit concentration would be 0.7 ppm.

For the final analysis, consider the finite catalytic conversion of C7H14 and CH4 in a monolith: mcase = 5

$$zzcharhc6c7_{jcase+1} = \frac{Rehc6_{jcase+1} \cdot Sc7T(Thc_{jcase+1}) \cdot dcell6}{2}$$

$$\frac{Lhc}{zzcharhc6c7_{mcase}} = 0.8137$$

$$zzcharhc6c1_{jcase+1} = \frac{Rehc6_{jcase+1} \cdot Sc1T(Trecin_{jcase+1}) \cdot dcell6}{2}$$

$$\frac{Lhc}{zzcharhc6c1_{mcase}} = 2.8064$$

$$nz = 400$$

$$Lhc = 8.89 \cdot \text{cm}$$

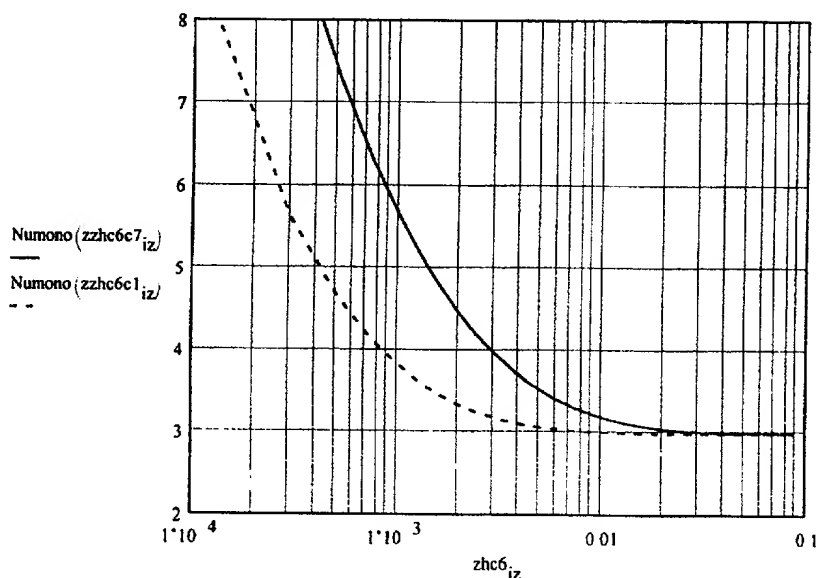
$$dcell6 = 0.0961 \cdot \text{cm}$$

$$zhc6_{iz} = iz \cdot \frac{Lhc}{nz} + dwall6$$

$$zzhc6c7_{iz} = \frac{zhc6_{iz}}{zzcharhc6c7_{mcase}}$$

$$zzhc6c1_{iz} = \frac{zhc6_{iz}}{zzcharhc6c1_{mcase}}$$

$$zzcharhc6c7 = \begin{bmatrix} 0 \\ 2.8414 \\ 3.6938 \\ 4.461 \\ 5.3986 \\ 10.926 \end{bmatrix} \cdot \text{cm}$$



Case specific mcase = 5

$$kgpblhc6c7(T, z) = \frac{Dc7h14T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc6c7_{mcase}}\right)}{dcell6}$$

$$kgpblhc6c7(Thc_{mcase}, Lhc) = 13.6172 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kgpblhc6c1(T, z) = \frac{Dch4T(T) \cdot \text{Numono}\left(\frac{z}{zzcharhc6c1_{mcase}}\right)}{dcell6}$$

$$kgpblhc6c1(Thc_{mcase}, Lhc) = 46.9581 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc6c1(T, z) = \frac{1}{\left(\frac{1}{\text{RatekCH4}(kpd(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc6c1(T, z)}}$$

$$kgpblhc6c1\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 46.9589 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc6c1\left(Thc_{mcase}, \frac{Lrec}{2}\right) = 1.8693 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{RatekCH4}(kpd(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 1.9467 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$keffhc6c7(T, z) = \frac{1}{\left(\frac{1}{\text{RatekC7H14}(2 \cdot ktpdC3(T), T) \cdot Lcat}\right) + \frac{1}{kgpblhc6c7(T, z)}}$$

$$kgpblhc6c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 13.6468 \cdot \text{sec}^{-1} \cdot \text{cm}$$

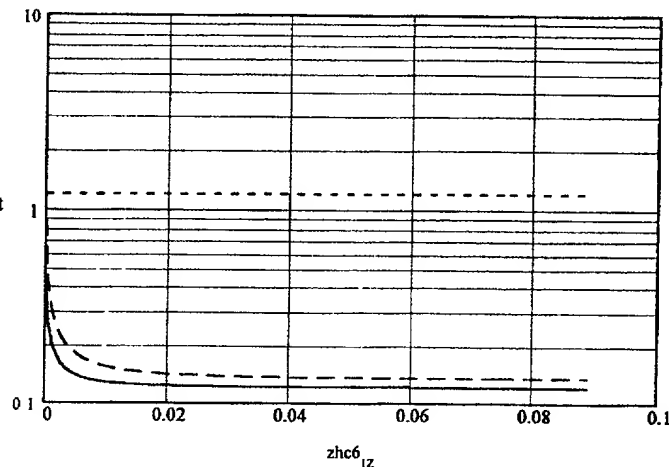
$$keffhc6c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 12.2537 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{RatekC7H14}(2 \cdot ktpdC3(Thc_{mcase}), Thc_{mcase}) \cdot Lcat = 120.0371 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\frac{keffhc6c7(Thc_{mcase}, zhc6_{iz})}{\text{RatekC7H14}(2 \cdot ktpdC3(Thc_{mcase}), Thc_{mcase}) \cdot Lcat}$$

$$= \frac{kgpbl6c7(Thc_{mcase}, zhc6_{iz})}{\text{RatekC7H14}(2 \cdot ktpdC3(Thc_{mcase}), Thc_{mcase}) \cdot Lcat}$$

$$= \frac{kgpbl6c7(Thc_{mcase}, zhc6_{iz})}{\text{RatekC7H14}(2 \cdot ktpdC3(Thc_{mcase}), Thc_{mcase}) \cdot Lcat}$$



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific

mcase = 5

$$yzkhc6c7h14_0 - yc7h140$$

$$yzkhc6ch4_0 - ych40$$

$$yzkhc6c7h14_{iz+1} = \left(1 - keffhc6c7(Thc_{mcase}, zhc6_{iz}) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell6} \cdot \frac{\epsilon_{cell6}}{Uhc6_{mcase}} \right) \cdot yzkhc6c7h14_{iz}$$

$$yzkhc6ch4_{iz+1} = \left(1 - keffhc6c1(Thc_{mcase}, zhc6_{iz}) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell6} \cdot \frac{\epsilon_{cell4}}{Uhc6_{mcase}} \right) \cdot yzkhc6ch4_{iz}$$

$$Thc = \begin{bmatrix} 0 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 916.4833 \end{bmatrix} \cdot K$$

Case specific

mcase = 5

$$yzkhc6c7h14_{nz} = 9.964 \cdot 10^{-6}$$

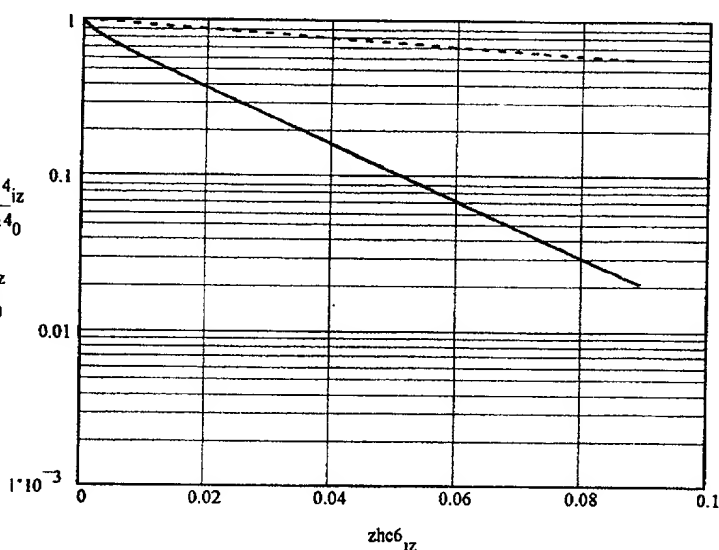
$$yzkhc6c7h14_0 = 0.0005$$

$$yzkhc6ch4_{nz} = 0.0028$$

$$yzkhc6ch4_0 = 0.005$$

$$\frac{yzkhc6c7h14_{nz}}{yzkhc6c7h14_0} = 1.993 \cdot 10^{-2}$$

$$\frac{yzkhc6ch4_{nz}}{yzkhc6ch4_0} = 0.5693$$



Case specific mcase = 5

Conversion of C7H14 under case 5 (full power) with 600 cells/in² x 3.5-in length and extrapolated catalytic rates (via C3H8 at 400C) is 98.0% [vs. 99.6% via averaged integrated formulas, 99.3% with temperature dependent transport, and 98.6% with 400 cells/in² and 4-in length. Conversion of CH4 is limited by slow kinetics and CO is expected to be very high (>99.99%).

Gas Properties and Constants

$$\begin{aligned} \text{cm} &\equiv 0.01 \cdot \text{m} & J &\equiv \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} & W &\equiv \text{J} \cdot \text{sec}^{-1} & \text{Pref} &= 1 \cdot \text{atm} \\ N &\equiv \text{kg} \cdot \text{m} \cdot \text{sec}^{-2} & \text{Pa} &\equiv \text{N} \cdot \text{m}^{-2} & \text{atm} &\equiv 101300 \cdot \text{Pa} & \mu\text{m} &\equiv 0.000001 \cdot \text{m} \\ R &= 8.3143 \cdot \frac{\text{J}}{\text{K}} & R_c &= 8.3143 \cdot \text{J} \cdot \text{mole}^{-1} \cdot \text{K}^{-1} \end{aligned}$$

n	Gas	MolWt	$\sigma(\text{LJ})$	$\epsilon(\text{LJ})$
1	CH4	$\text{MW}_0 = 16.044 \cdot \text{gm}$	$\sigma_0 = 3.785 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_0 = 148.6 \cdot \text{K}$
2	O2	$\text{MW}_1 = 31.999 \cdot \text{gm}$	$\sigma_1 = 3.464 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_1 = 106.7 \cdot \text{K}$
3	N2	$\text{MW}_2 = 28.018 \cdot \text{gm}$	$\sigma_2 = 3.798 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_2 = 71.4 \cdot \text{K}$
4	CO2	$\text{MW}_3 = 44.010 \cdot \text{gm}$	$\sigma_3 = 3.941 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_3 = 195.2 \cdot \text{K}$
5	H2O	$\text{MW}_4 = 18.015 \cdot \text{gm}$	$\sigma_4 = 2.641 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_4 = 809.1 \cdot \text{K}$

Define transport integrals:

Constants:

$$\begin{aligned} \sigma\mu a_0 &= 1.16145 & \sigma\mu b_0 &= 0.14874 & \sigma D a_0 &= 1.06036 & \sigma D b_0 &= 0.1561 \\ \sigma\mu a_1 &= 0.52487 & \sigma\mu b_1 &= 0.7732 & \sigma D a_1 &= 0.193 & \sigma D b_1 &= 0.47635 \\ \sigma\mu a_2 &= 2.16178 & \sigma\mu b_2 &= 2.43787 & \sigma D a_2 &= 1.03587 & \sigma D b_2 &= 1.52996 \\ & & & & \sigma D a_3 &= 1.76474 & \sigma D b_3 &= 3.89411 \end{aligned}$$

Functions:

$$\Omega\mu(T) = \sigma\mu a_0 \cdot \exp[-(\sigma\mu b_0 \cdot \ln(T))] + \sum_{i\mu=1}^2 \sigma\mu a_{i\mu} \cdot \exp(-\sigma\mu b_{i\mu} \cdot T) \quad \Omega\mu(3) = 1.0394$$

$$\Omega D(T) = \sigma D a_0 \cdot \exp[-(\sigma D b_0 \cdot \ln(T))] + \sum_{iD=1}^3 \sigma D a_{iD} \cdot \exp(-\sigma D b_{iD} \cdot T) \quad \Omega D(3) = 0.95002$$

B5
B4

Set Inlet Conditions:

$$P = 1.0\text{-atm} \quad y_{ch40} = 0.035$$

Define gas composition w/r methane using moist (3%) air:

$$y(x) = \begin{bmatrix} x \\ (1 - y_{ch40}) \cdot 0.2 - 2 \cdot y_{ch40} + 2 \cdot x \\ (1 - y_{ch40}) \cdot 0.77 \\ y_{ch40} - x \\ (1 - y_{ch40}) \cdot 0.03 + 2 \cdot y_{ch40} - 2 \cdot x \end{bmatrix} \quad y(0.02) = \begin{bmatrix} 0.02 \\ 0.163 \\ 0.743 \\ 0.015 \\ 0.059 \end{bmatrix}$$

Define viscosity function

$$\mu(T) = \begin{bmatrix} \frac{2.6693 \cdot 10^{-26} \cdot (MW_0 \cdot T)^{0.5}}{(\sigma_0)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_0} \right)} \cdot \frac{10^5 \cdot \text{cm}}{\text{sec}} \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \\ \frac{(MW_1 \cdot T)^{0.5}}{(\sigma_1)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_1} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \\ \frac{(MW_2 \cdot T)^{0.5}}{(\sigma_2)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_2} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \\ \frac{(MW_3 \cdot T)^{0.5}}{(\sigma_3)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_3} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \\ \frac{1.116 \cdot (MW_4 \cdot T)^{0.5}}{(3.115 \cdot 10^{-8} \cdot \text{cm})^2 \cdot \Omega \mu \left(\frac{T}{514 \cdot \text{K}} \right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot \text{cm}}{\text{sec}} \right) \cdot \left(\frac{\text{gm}}{\text{K}} \right)^{0.5} \right] \end{bmatrix} \quad \mu(300 \cdot \text{K}) = \begin{bmatrix} 1.103 \cdot 10^{-5} \\ 2.06 \cdot 10^{-5} \\ 1.77 \cdot 10^{-5} \\ 1.519 \cdot 10^{-5} \\ 1.068 \cdot 10^{-5} \end{bmatrix} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

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$$\mu_{\text{mix}}(x, T) = \frac{\sum_{n=0}^4 y(x)_n \cdot (\mu(T))_n}{\sum_{m=0}^4 y(x)_m \cdot \frac{\left[1 + \left(\frac{\mu(T)_n}{\mu(T)_m} \right)^{0.5} \cdot \left(\frac{MW_m}{MW_n} \right)^{0.25} \right]^2}{\left[8 \cdot \left(1 + \frac{MW_n}{MW_m} \right) \right]^{0.5}}}}$$

$$y(0.02) = \begin{bmatrix} 0.02 \\ 0.163 \\ 0.743 \\ 0.015 \\ 0.059 \end{bmatrix}$$

$$\mu_{\text{mix}}(0.02, 300 \cdot K) = 1.759 \cdot 10^{-5} \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-1}$$

Define thermal conductivity functions

igas = 0, 1..4

$$a\lambda = \begin{bmatrix} -1.869 \\ -3.273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda = \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda = \begin{bmatrix} 1.179 \cdot 10^{-4} \\ -(3.743 \cdot 10^{-5}) \\ -(5.067 \cdot 10^{-5}) \\ 5.477 \cdot 10^{-6} \\ 1.801 \cdot 10^{-4} \end{bmatrix} \quad d\lambda = \begin{bmatrix} -(3.614 \cdot 10^{-8}) \\ 9.732 \cdot 10^{-9} \\ 1.504 \cdot 10^{-8} \\ -(1.053 \cdot 10^{-8}) \\ -(9.1 \cdot 10^{-8}) \end{bmatrix}$$

CH4
O2
N2
CO2
H2O

$$\lambda(i, T) = \left[a\lambda_i + b\lambda_i \frac{T}{K} + c\lambda_i \left(\frac{T}{K} \right)^2 + d\lambda_i \left(\frac{T}{K} \right)^3 \right] \cdot 0.00001 \cdot \frac{W}{\text{cm} \cdot K} \quad W/\text{cm} \cdot K$$

$$\lambda_{\text{mix}}(x, T) = \frac{\sum_{i=0}^4 y(x)_i \cdot \lambda(i, T)}{\sum_{j=0}^4 y(x)_j \cdot \frac{\left[1 + \left(\frac{\mu(T)_i}{\mu(T)_j} \right)^{0.5} \cdot \left(\frac{MW_j}{MW_i} \right)^{0.25} \right]^2}{\left[8 \cdot \left(1 + \frac{MW_i}{MW_j} \right) \right]^{0.5}}}}$$

$\lambda(\text{igas}, 1000 \cdot K)$

0.16716 · kg · m · sec ⁻³ · K ⁻¹
0.07163 · kg · m · sec ⁻³ · K ⁻¹
0.06292 · kg · m · sec ⁻³ · K ⁻¹
0.06788 · kg · m · sec ⁻³ · K ⁻¹
0.08631 · kg · m · sec ⁻³ · K ⁻¹

$$\lambda_{\text{mix}}(.0, 1000 \cdot K) = 6.64 \cdot 10^{-4} \cdot \frac{W}{\text{cm} \cdot K}$$

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Define thermal conductivity of alumina and SS321

$$\text{Alt}c = \begin{bmatrix} 83.71 \\ 224.898 \\ 255.842 \\ 132.727 \\ 25.9695 \end{bmatrix}$$

The parameter set Alt_c_n was determined from published values of the thermal conductivity. Ref: HCP

$\lambda_{\text{Al2O3}}(x)$ is the thermal conductivity function (of x with unit K) while λ_1 is its derivative w/r to temperature.

$$\lambda_{\text{Al2O3}}(x) = \sum_{n=0}^4 \text{Alt}c_n \cdot \left(\frac{x}{1000 \cdot K}\right)^n \cdot \frac{W}{m \cdot K} \quad \lambda_1(x) = \sum_{n=1}^4 \frac{\text{Alt}c_n}{1000 \cdot K} \cdot n \cdot \left(\frac{x}{1000 \cdot K}\right)^{n-1} \cdot \frac{W}{m \cdot K}$$

$$\text{S321tc} = \begin{bmatrix} 4.69312 \\ 4.9812 \\ -0.33357 \\ 0 \\ 0 \end{bmatrix}$$

The parameter set S321tc_n was determined from published values of the thermal conductivity. Ref: Handbook of Metals 8th Ed. Vol. 1 p. 423

$$\lambda_{\text{ss321}}(x) = \sum_{n=0}^4 \text{S321tc}_n \cdot \left(\frac{x}{1000 \cdot K}\right)^n \cdot \frac{W}{m \cdot K}$$

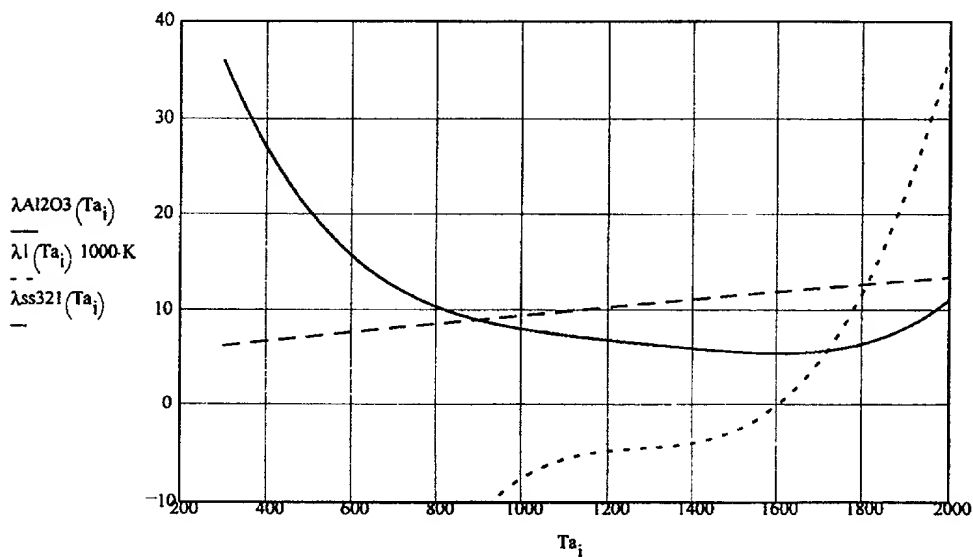
$$\lambda_{\text{ss321}}(1000 \cdot K) = 9.341 \cdot \frac{W}{m \cdot K}$$

$$\lambda_{\text{Al2O3}}(1000 \cdot K) = 7.897 \cdot \frac{W}{m \cdot K}$$

$$\lambda_1(1000 \cdot K) \cdot 1000 \cdot K = -7.517 \cdot \frac{W}{m \cdot K}$$

$$i = 30, 31 \dots 200$$

$$T_{a_i} = 10 \cdot i \cdot K$$



$$x_0 = 1.588 \cdot 10^3 \cdot \text{K}$$

$$0.003 \cdot \text{in} = 7.62 \cdot 10^{-3} \cdot \text{cm}$$

$$\lambda_{\text{Al}_2\text{O}_3}(200\cdot\text{K}) = 0.479 \cdot \frac{\text{W}}{\text{cm}\cdot\text{K}}$$

$$\lambda_{Al_2O_3(x)} = 0.054 \cdot \frac{W}{cm \cdot K}$$
 Minimum thermal conductivity

Ref: RHG - Handbook Chpt 6 for effective thermal conductivity including convection and radiative terms

$$dp = 5 \cdot 10^{-7} \cdot m$$

$$\lambda_{\text{wcr}}(x, T) = \lambda_{\text{mix}}(x, T) \cdot \left[0.0931 + 2 \cdot 0.9069 \cdot \left(\frac{\lambda_{\text{Al}_2\text{O}_3}(T)}{\lambda_{\text{Al}_2\text{O}_3}(T) - \lambda_{\text{mix}}(x, T)} \right)^2 \cdot \left(\ln \left(\frac{\lambda_{\text{Al}_2\text{O}_3}(T)}{\lambda_{\text{mix}}(x, T)} \right) - 1 \right) \right]$$

Radiation component negligible with such small particles in the washcoat

$$\lambda_{ss321}(1000\cdot K) = 9.341 \cdot \frac{W}{m \cdot K}$$

$$\frac{\lambda_{\text{Al}_2\text{O}_3}(1000\cdot\text{K})}{\lambda_{\text{mix}}(0.01, 1000\cdot\text{K})} = 117.74$$

$$\frac{\lambda_{\text{wc}}(0.01, 1000\cdot\text{K})}{\lambda_{\text{mix}}(0.01, 1000\cdot\text{K})} = 7.046$$

The thermal conductivity of the wash coat is about 7 times greater at 1000K than the gas phase conductivity

$$\frac{\lambda_{\text{wc}}(0.01, 1000\cdot\text{K})}{\lambda_{\text{ss321}}(1000\cdot\text{K})} = 0.051$$

$$\frac{\frac{\lambda_{\text{wc}}(0.01, 1000\cdot\text{K})}{0.001\cdot\text{cm}} + \frac{\lambda_{\text{ss321}}(1000\cdot\text{K})}{0.003\cdot\text{in}}}{\frac{\lambda_{\text{ss321}}(1000\cdot\text{K})}{0.003\cdot\text{in}}} = 1.386$$

The washcoat increases the thermal conductance of the wall by about 39%

$$\frac{\lambda_{\text{ss321}}(1000\cdot\text{K})}{\lambda_{\text{mix}}(0.01, 1000\cdot\text{K})} = 139.275$$

For a Nusselt no. of 2.976 ($d_{\text{cell}} = 0.0961\cdot\text{cm}$) for developed flow in the recuperator (full power) the mean heat transfer boundary layer thickness is much greater than either the SS321 wall thickness or the washcoat thickness.

$$\delta_{\text{gprecup}} = \frac{0.0961\cdot\text{cm}}{2.976}$$

$$\delta_{\text{gprecup}} = 0.032\cdot\text{cm}$$

$$h_{\text{recavg}}(T) = \frac{1}{\left(\frac{2}{\lambda_{\text{mix}}(0.01, T)} \right) \frac{1}{\delta_{\text{gprecup}}} + \frac{1}{\lambda_{\text{ss321}}(1000\cdot\text{K})} \frac{1}{0.003\cdot\text{in}}}$$

Overall local heat transfer coefficient for the recuperator (assuming gas phase conductivities are about the same)

$$h_{\text{recavgwc}}(T) = \frac{1}{\left[\frac{1}{\lambda_{\text{mix}}(0.01, T)} \frac{1}{\delta_{\text{gprecup}} - \frac{2\cdot 0.001\cdot\text{cm}}{2.976}} \right] + \left(\frac{1}{\lambda_{\text{mix}}(0.01, T)} \frac{1}{\delta_{\text{gprecup}}} \right) + \left(\frac{1}{\lambda_{\text{ss321}}(1000\cdot\text{K})} \frac{1}{0.003\cdot\text{in}} \right) + \frac{\text{Effect of wash coat on heat transfer coefficient}}{\lambda_{\text{wc}}(0.01, T) \frac{1}{0.001\cdot\text{cm}}}}$$

$$h_{\text{recavg}}(1000\cdot\text{K}) = 0.01038 \cdot \frac{\text{W}}{\text{cm}^2\cdot\text{K}}$$

$$h_{\text{recavgwc}}(1000\cdot\text{K}) = 0.01046 \cdot \frac{\text{W}}{\text{cm}^2\cdot\text{K}}$$

The wash coat makes about 0.1% increase in heat transfer coefficient because of the slightly decreased cell size and greater thermal conductivity of the washcoat vs. gas phase.

APPENDIX C

COMBUSTION CATALYSTS FOR TURBINES

Introduction

I described possible alternative combustion catalyst configurations and detailed analysis of relevant performance factors, i.e., mass-transfer limited hydrocarbon conversions, pressure drop, catalyst temperatures, post combustion conversion of hydrocarbons and CO, etc. This report represents a comprehensive collection of my findings and comments. Attached are the final MathSoft Mathcad 6 analyses of the suggested alternative combustion catalyst configurations.

Alternative Combustion Catalyst Configurations

Two approaches are suggested for the catalytic combustion of gasoline vapors in air. These approaches represent more conventional and perhaps less expensive alternatives to the PCI Microlith™ technology. They are summarized as follows:

- **Monolith with bypass air** -- A standard 3.5", corrugated FeCrAl alloy, 600 cells/in² monolith should be able to reach $\approx 86\%$ (naphtha) to $>99.8\%$ (natural gas) fuel conversions. Using an air by-pass would allow longer residence time and higher adiabatic temperature rise (which is probably necessary for natural gas but may not be for diesel fuel or naphtha) within the combustor to ensure fast catalytic reaction rates. Higher temperatures within and at the exit of the catalyst monolith would also increase homogeneous combustion reactions, and help convert residual fuel vapors in the region immediately downstream of the catalyst but upstream of the turbine. A controller for bypass flow could help with turn-down, startup, and tuning steady-state conversions.
- **Radial flow catalyst bed** -- Provided that the flow rate can be reduced to < 3 m/s, a thin packed bed of catalyst beads or granules may also achieve conversions similar to those of the monolith and PCI Microlith™ catalyst screens at equivalent pressure drop. The bed might intrude upon your fuel injection and premixing zone, but this could actually benefit combustion (within limits, e.g., $\pm 30\%$ fuel/air ratio) by providing locally higher adiabatic temperatures. A packed bed has fairly good thermal conductivity and is virtually immune to thermal shock problems. A screened frame and possibly metal plates (or alternatively for robustness, silica-coated silicon carbide) could be located within the bed to guide the flow. Downstream hydrocarbon and CO conversion also would be necessary for low emissions as in the case of the monolith.

- **Exhaust converter** -- A 400 cells/in² post combustion monolith located just ahead of the regenerator exhaust stream inlet could provide a very significant reduction in hydrocarbon emissions regardless of the configuration and performance of the combustion catalyst. An emission control monolith should remove about 99% of the residual unburned fuel components and > 99.9% of the CO.
- [REDACTED]

Analysis of Catalyst Performance

Mathsoft's Mathcad 6.0 Plus Professional program was used to perform detailed calculations of pressure drop and conversion of C₁, C₅, C₇, and C₉ hydrocarbons (methane, isopentane, cycloheptane and nonene) and CO. The analyses generally assume catalytic rates are fast under Capstone's specified combustion conditions. The analyses use various catalyst parameters such as particle/channel size and bed length for the two upstream (monolith and fixed bed) configurations. Only monoliths were considered for the downstream 1-atm conversion of residual CO and hydrocarbons.

Gas Properties

Initially the Mathcad document describes and defines various gas component and mixture properties and functions (pp. 1-13) that are used in the subsequent calculations. The gas and vapor components are identified with their physical parameters (p. 1) and the composition of combustion mixtures as a function of fuel conversion are defined (pp. 2-3). Mixture densities, diffusivities of individual fuel component in the mixtures, viscosity, and thermal conductivity are then defined and plotted as functions of composition and temperature (pp. 4-9). The composition of various fuel mixtures is shown to minimally effect mixture physical properties (< 0.5% under such lean conditions). These properties are then redefined as empirical functions of temperature for simplification of subsequent analysis (pp. 6-9). Heat capacities, heats of combustion and enthalpy functions of the mixtures are similarly defined (pp. 9-11), and the initial composition necessary for

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an adiabatic temperature rise of 511°F are determined for each of the four fuel components (p. 11 and re-entered on p. 2). Finally, transport functions, e.g., Prandtl Number, Schmidt Number, thermal diffusivity, momentum diffusivity, etc., are defined (pp. 12-13) prior to definitions of the catalyst configurations, geometry, and flow conditions.

Catalyst Configurations

The physical parameters of several catalyst configurations (honeycomb monoliths and packed beds) and the appropriate flow conditions are described (p. 14) and used in the subsequent analyses.

Combustion Monolith Performance

The pressure drop values for (standard) 3.5 or 4.0 inch length 400 and 600 cells/in² monoliths are determined as functions of flow rate (pp. 15-16, and see figure on p. 16). Heat and mass Nusselt functions are defined and used to calculate single-pass fuel conversion vs. monolith depth (p. 17-19). It is possible to determine laminar flow hydrothermal Nusselt functions for square or sinusoidal channels (which may be more representative of actual monolith channel shapes), but this was not included in the current analysis. Accordingly the Nusselt functions cannot be considered more accurate than about $\pm 30\%$.

The results of the performance analysis for the monoliths are summarized in a table (p. 18) for the two cell densities, the two lengths, and 0, 20, and 40% by-pass air. The transport-limiting conversion of fuel components is plotted as a function of pressure drop for constant flow rate but extended monolith length (p. 19). High fuel conversions ($\approx 99.5\%$) are possible with the 600 cells/in² monolith at 1% pressure drop (but it requires 10 inches length).

Post Combustion Converter

Analysis of post-combustion downstream (1-atm vs. 3-atm upstream) conversion of CO and fuels and the pressure drop in 400 and 600 cpi monoliths shows excellent results for such a wide area monolith (pp. 20-25). After defining component diffusivity functions and describing monolith configuration (pp. 20-21), the pressure drop and conversions of CO and fuel vapors are calculated and plotted as functions of monolith depth (pp. 21-23). Finally, the results of an analysis of the overall conversions of individual hydrocarbons and CO including upstream combustor, homogeneous combustion, and the exhaust converter are tabulated (p. 23).

Differential (Local) Nusselt Analysis

A different analysis, where the local hydrothermal Nusselt functions are defined and integrated over the length of a monolith (pp. 24-25), are used to check the integral formulas.

These values (p. 25), which are derived from different sources (Kays and Crawford, "Convection Heat and Mass Transfer," 3rd, 1993, vs. Rosner, "Transport Processes in Chemically Reacting Systems", 1986) show higher conversions than the integrated values, e.g., 94% conversion for C_7H_{14} vs. 86% with the integral expression. This difference appears to be caused by the greater effect of hydrothermal entrance (as opposed to hydrodynamically developed flow with thermal entrance) and shows the integral formulas to be conservative by a factor of about two.

Combustion with Packed Beds

Pressure drop and fuel conversion functions are defined and used to analyze the performance of packed beds (pp. 26-31). Pressure drop is a strong function of the superficial flow rate, nearly second order (pressure drops are calculated and plotted against superficial linear flow velocity for various sizes of catalyst particles on p. 27). Gas to particle Nusselt numbers for packed beds are developed plotted for methane, isopentane, cycloheptane and nonene for three sizes of catalyst granules (pp. 27-28). Shape factors are not included in this analysis, so the results represent values for packed spheres with equivalent effect on ΔP , not with equivalent diameter. The conversion of fuel components (again assuming very fast catalytic rates) is determined (pp. 28-29) for the oblique flow geometry (which is defined on p. 16).

For full perpendicular flow such as with an annular cylindrical packed bed rather than the conical bed, the pressure drop function is much greater for equivalent conversion of fuel components. This is caused by the higher power dependence of ΔP on flow velocities (form drag), while the conversion per unit depth of bed increases almost linearly with increasing flow rate. At flows higher than about 2 m/s the catalyst granules begin to act as bluff bodies which cause the flow to accelerate around them. While this increases backmixing which helps convection, it causes a greater effect on the pressure drop. Conversions for methane and cycloheptane are plotted as a function of pressure drop for beds of 1-mm and 1/8-in. granules (pp. 29-31). For oblique flow (2.5 m/s superficial velocity through the conical bed) with the small granules, C_7H_{14} conversions are calculated to be very high ($> 99.99\%$) at 1% pressure drop, while for perpendicular flow (8.2 m/s) with the 1/8-in. pellets, C_7H_{14} conversions are calculated to be very low ($\approx 62\%$) at 2% pressure drop. Clearly some radial configuration must be used to achieve high conversions with the packed beds without a pressure drop penalty.

Required Catalytic Rates

Finally, the specific catalytic rate constants required for conversions of methane and cycloheptane in a 600 cells/in² monolith are determined (pp. 32-35) for Capstone's conditions.

Table 1. Demographic characteristics of the study population	
Age (years)	Mean (SD)
18-24	20.5 (2.5)
25-34	29.5 (4.5)
35-44	39.5 (5.5)
45-54	49.5 (6.5)
55-64	59.5 (7.5)
65-74	69.5 (8.5)
75-84	79.5 (9.5)
85-94	89.5 (10.5)
95-104	99.5 (11.5)
105-114	109.5 (12.5)
115-124	119.5 (13.5)
125-134	129.5 (14.5)
135-144	139.5 (15.5)
145-154	149.5 (16.5)
155-164	159.5 (17.5)
165-174	169.5 (18.5)
175-184	179.5 (19.5)
185-194	189.5 (20.5)
195-204	199.5 (21.5)
205-214	209.5 (22.5)
215-224	219.5 (23.5)
225-234	229.5 (24.5)
235-244	239.5 (25.5)
245-254	249.5 (26.5)
255-264	259.5 (27.5)
265-274	269.5 (28.5)
275-284	279.5 (29.5)
285-294	289.5 (30.5)
295-304	299.5 (31.5)
305-314	309.5 (32.5)
315-324	319.5 (33.5)
325-334	329.5 (34.5)
335-344	339.5 (35.5)
345-354	349.5 (36.5)
355-364	359.5 (37.5)
365-374	369.5 (38.5)
375-384	379.5 (39.5)
385-394	389.5 (40.5)
395-404	399.5 (41.5)
405-414	409.5 (42.5)
415-424	419.5 (43.5)
425-434	429.5 (44.5)
435-444	439.5 (45.5)
445-454	449.5 (46.5)
455-464	459.5 (47.5)
465-474	469.5 (48.5)
475-484	479.5 (49.5)
485-494	489.5 (50.5)
495-504	499.5 (51.5)
505-514	509.5 (52.5)
515-524	519.5 (53.5)
525-534	529.5 (54.5)
535-544	539.5 (55.5)
545-554	549.5 (56.5)
555-564	559.5 (57.5)
565-574	569.5 (58.5)
575-584	579.5 (59.5)
585-594	589.5 (60.5)
595-604	599.5 (61.5)
605-614	609.5 (62.5)
615-624	619.5 (63.5)
625-634	629.5 (64.5)
635-644	639.5 (65.5)
645-654	649.5 (66.5)
655-664	659.5 (67.5)
665-674	669.5 (68.5)
675-684	679.5 (69.5)
685-694	689.5 (70.5)
695-704	699.5 (71.5)
705-714	709.5 (72.5)
715-724	719.5 (73.5)
725-734	729.5 (74.5)
735-744	739.5 (75.5)
745-754	749.5 (76.5)
755-764	759.5 (77.5)
765-774	769.5 (78.5)
775-784	779.5 (79.5)
785-794	789.5 (80.5)
795-804	799.5 (81.5)
805-814	809.5 (82.5)
815-824	819.5 (83.5)
825-834	829.5 (84.5)
835-844	839.5 (85.5)
845-854	849.5 (86.5)
855-864	859.5 (87.5)
865-874	869.5 (88.5)
875-884	879.5 (89.5)
885-894	889.5 (90.5)
895-904	899.5 (91.5)
905-914	909.5 (92.5)
915-924	919.5 (93.5)
925-934	929.5 (94.5)
935-944	939.5 (95.5)
945-954	949.5 (96.5)
955-964	959.5 (97.5)
965-974	969.5 (98.5)
975-984	979.5 (99.5)
985-994	989.5 (100.5)
995-1004	999.5 (101.5)
1005-1014	1009.5 (102.5)
1015-1024	1019.5 (103.5)
1025-1034	1029.5 (104.5)
1035-1044	1039.5 (105.5)
1045-1054	1049.5 (106.5)
1055-1064	1059.5 (107.5)
1065-1074	1069.5 (108.5)
1075-1084	1079.5 (109.5)
1085-1094	1089.5 (110.5)
1095-1104	1099.5 (111.5)
1105-1114	1109.5 (112.5)
1115-1124	1119.5 (113.5)
1125-1134	

[REDACTED]

Conclusions

Several conclusions can be drawn about the transport limiting performance of a catalysts used to combustion gasoline and methane fuels for Capstone's 24 kW microturbine:

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modest conversion for gasoline (94% for cycloheptane) etc. with low pressure drop.

- 2) If the fuel air mixing can be moved upstream sufficiently to allow use of a longer catalyst monoliths, significantly lower emission could result without unacceptable ($> 1\%$) pressure drop ratio. For $1\% \Delta P/P$ drop (with greater monolith length), transport limited conversion of C_7H_{14} should reach 99.5% in an active 600 cells/in² honeycomb monolith.
- 3) Post combustion monolith catalysts should be considered for use in EZEV turbines, regardless of the method of fuel conversion during combustion. A short 400 cells/in² Alpha-IV metal monolith coated with a layer of supported Pt located at the inlet to the recuperator can give very significant emission reductions for CO and all hydrocarbons because of the lower linear velocities, high exhaust temperature, greater diffusivities at 1-atm. Conversions of CO and CH_4 can be very high, while conversions with C_7H_{14} and other gasoline fuels is less, it still can bring the gasoline range fuel components in the exhaust to a few ppm with the assumption that only a modest degree of homogeneous combustion occurs upstream of the turbine.
- 4) Provided that significant homogeneous combustion occurs within the channels and downstream of the monolith ($\approx 80\%$ conversion giving 60 ppm C_7H_{14} and 840 ppm CO leaving the turbine) and that a 400 cells/in² post combustion hydrocarbon oxidation catalyst was used downstream, gasoline emissions should fall below 0.5 ppm.
- 5) The oblique flow/conical catalyst packed bed could also be considered as an option to the MicrolithTM and honeycomb monolith catalysts. The performance of the packed beds can be very good in terms of fuel conversion with the smaller catalyst granules. Yet, these beds must have some element of radial flow as the pressure drop for a flow linear flow rate will cause excessive pressure drop. A word of caution here, packed beds are more susceptible to flash back caused by the higher degree of backmixing and regions where local residence times can be quite long relative to the screens and monoliths.

Catalyst Durability, Robustness, and Costs

- 1) [REDACTED] concerns were expressed about the tolerance of combustion catalysts to momentarily high fuel/air ratios and local unmixedness. While clearly high degrees of F/A control and uniformly premixed combustion gases are desired, the combustion catalysts should show robustness sufficient to survive short excursions of off-specification F/A ratio conditions as well as showing the durability necessary for long active life under normal operation at high temperatures.
- 2) The greater the thermal mass of the catalyst, the greater its robustness in the face of locally or globally high F/A. In this regard the packed beds would be

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superior to the fine screens of the Microlith™ and the thin walled metal monoliths.

- 3) A packed bed also has greater ability to disperse locally high F/A mixtures to a greater extent than the Microlith™ and to a much greater than the honeycomb channels. High thermal conductivity also improves robustness in locally high F/A (hot spot) conditions. Here the packed bed is perhaps superior to the metal monolith because of its greater radial conductivity, while the screens have very little ability (radiation) to disperse heat from locally hot zones.
- 4) The Alpha-IV alloy honeycomb should be much more resistant to fast overheating to high temperatures than the PCI microlith. The Alzeta/Grace electrically heated monolith previously examined by Capstone (Nomac) had entrance channels too large to give high conversion except with long length and smaller channels downstream, hence the large volume and weight.
- 5) Packed beds represent the least cost catalyst for combustion because they use configurations and materials common with commercial VOC incineration catalysts. The metal monoliths have low costs because of their widespread acceptance and increasing use in automobile catalytic converters and as VOC catalysts. The premixed, gasoline-fueled, and recuperated nature of the combustion process for Capstone's microturbines is a good fit (with a slight push to higher pressure, higher throughput, low pressure drop, and greater robustness) with the commercial VOC catalysts available from several sources, including Prototech/United Catalysts. It would not appear necessary to develop new catalyst and catalytic engineered combustors for Capstone' microturbine combustion applications.

The following table summarizes the findings of this analysis:

Property	Ranking		
Fuel Conversion	Packed Beds >	Screens >	Monoliths
Pressure Drop	Monoliths >	Screens >	Packed Beds
Durability	Packed Beds ≈	Monoliths ≈	Screens
Robustness	Packed Beds >	Monoliths >	Screens
Cost & Availability	Packed Beds >	Monoliths >	Screens

[REDACTED]

[REDACTED]

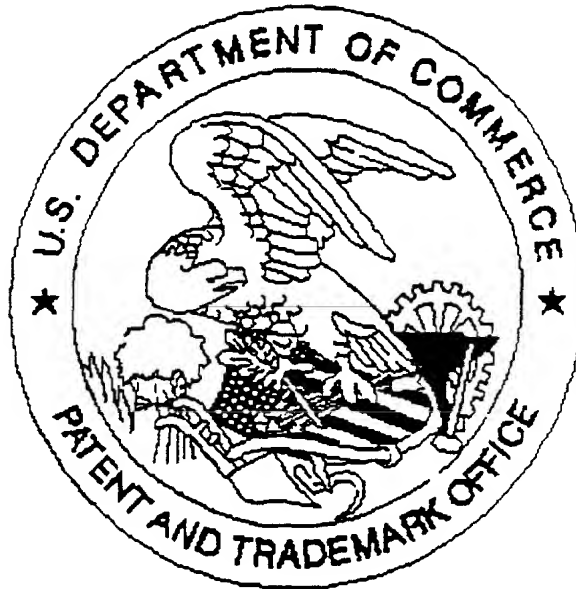
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Final Recommendations

Use of Catalysts in Existing Engines

The following recommendations are made on the basis of improving the *existing* microturbine catalytic combustion performance:

- 1) Install 400 cells/in² 1-atm monolith with a Pt-based catalyst for post combustion CO and hydrocarbon removal. This unit should provide the greatest improvement in emissions with little effect on pressure drop at modest cost (\approx \$200/unit installed). It could be used with all catalytic and even with non-catalytic burners to reduce CO and hydrocarbon emissions. However, it cannot be effective in reducing NOx emissions from non-catalytic burners.
- 2) Use a 600 cells/in² Alpha-IV alloy metal monolith of 4-in. length with premixed fuel and air as a lower pressure drop alternative to the PCI Microlith™ system. Fuel conversion may be lower than the PCI unit, but with lower pressure drop; at equivalent $\Delta P/P$, the monolith should show superior fuel conversion. A small amount of by-pass air could help with turn-down and could be used to improve emissions during normal operation by increasing residence time and allowing higher temperatures in the homogeneous zones within the channels and immediately downstream of the combustor.

Use of Catalysts in Advanced Engines

For *advanced* combustion systems, the fuel air mixing could be moved upstream of its current position to allow great premixing and to give greater volume for the catalyst.

- 1) Nominally 1-mm to 1/16-in. packed beds in a conical configuration with about 2-3 m/s linear superficial bed velocity could give good performance, especially with a small bypass air stream for post catalyst hydrocarbon reduction. An inconel screen could be located upstream to suppress flashback and ceramic foams or honeycomb monoliths could be used as mechanical supports to increase robustness.
- 2) A longer 600 cells/in² Alpha-IV alloy metal monolith (from 3.5- to 8- or 10-in.) could also decrease hydrocarbon and CO emissions with acceptable $\Delta P/P$ by relocating the F/A mixing zone upstream.

Additional Catalytic R&D Activities

Additional Analysis -- Fuel combustion rates can be measured for specific catalysts under Capstone's combustion conditions. The rates can be incorporated in an extended analysis of

combustor performance for use in predicting fuel conversion, specifying required catalyst activity maintenance (e.g., Is it close to extinction at 1000°F inlet temperature?), and assisting in the design of current and next generation combustors (e.g., How much by-pass air is necessary? What are the limited on F/A ratios?, etc.).

Advanced Materials

more robust units could be developed with ceramic structural components and state-of-the-art catalysts capable of resisting short (a few seconds) temperature excursions to 3000°F (1650°C). The attrition resistance and crush strength of the Norton SA 6576 catalyst pellets supplied to Capstone by SRI International also need improvement (their very large specific volume of macropores, while desirable, leads to poor mechanical strength), and other catalysts (e.g., 1.5-mm extruded, Pt-promoted, Mn-substituted hexa-aluminates) could be examined for activity and attrition resistance.

In the longer-term,

SRI could coat steels with chromium and aluminum (*in situ* preparation of FeCrAl alloy films) to prepare inexpensive, high-performance recuperators and monoliths for use in advanced higher temperature engines.

Systems -- Additional engineering analysis and catalyst preparation and testing could provide Capstone with cost effective assistance in the design of EZEV turbogenerators with alternative fuels such as LPG, CNG, and diesel for hybrid vehicles. LPG could be used in the current designs with combustion and exhaust converter monoliths; CNG could be used with combustion and exhaust converter monoliths, but with by-pass air to increase F/A ratios and catalyst temperatures; and diesel fuel could require upstream mixing with long combustion monoliths or conical beds and longer exhaust converter monoliths.

Appendix C

CAPSTONE MOL

Gas Properties and Constants

$$\begin{aligned} \text{cm} &= 0.01 \cdot \text{m} & J &= \text{kg} \cdot \text{m}^2 \cdot \text{sec}^{-2} & W &= J \cdot \text{sec}^{-1} & \text{Pref} &= 1 \cdot \text{atm} \\ N &= \text{kg} \cdot \text{m} \cdot \text{sec}^{-2} & \text{Pa} &= \text{N} \cdot \text{m}^{-2} & \text{atm} &= 101300 \cdot \text{Pa} & \mu\text{m} &= 0.000001 \cdot \text{m} \\ R &= 8.3143 \cdot \frac{J}{K} & R_c &= 8.3143 \cdot J \cdot \text{mole}^{-1} \cdot K^{-1} \end{aligned}$$

n	Gas	MolWt	$\sigma(\text{LJ})$	$\epsilon(\text{LJ})$
1	CH ₄	$MW_0 = 16.044 \cdot \text{gm}$	$\sigma_0 = 3.785 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_0 = 148.6 \cdot \text{K}$
2	O ₂	$MW_1 = 31.999 \cdot \text{gm}$	$\sigma_1 = 3.464 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_1 = 106.7 \cdot \text{K}$
3	N ₂	$MW_2 = 28.018 \cdot \text{gm}$	$\sigma_2 = 3.798 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_2 = 71.4 \cdot \text{K}$
4	CO ₂	$MW_3 = 44.010 \cdot \text{gm}$	$\sigma_3 = 3.941 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_3 = 195.2 \cdot \text{K}$
5	H ₂ O	$MW_4 = 18.015 \cdot \text{gm}$	$\sigma_4 = 2.641 \cdot 10^{-10} \cdot \text{m}$	$\epsilon_4 = 809.1 \cdot \text{K}$

6 C₅H₁₂
2-methyl-butane

$$\begin{aligned} T_{b5} &= 301 \cdot \text{K} & T_{c5} &= 460.4 \cdot \text{K} & P_{c5} &= 3.39 \cdot 10^6 \cdot \text{Pa} & V_{c5} &= 306 \\ \epsilon_5 &= \frac{T_{c5}}{1.2593} & \sigma_5 &= V_{c5}^{\frac{1}{3}} \cdot 10^{-10} \cdot \text{m} \\ MW_5 &= 72.151 \cdot \text{gm} & \epsilon_5 &= 365.59994 \cdot \text{K} & \sigma_5 &= 6.73866 \cdot 10^{-10} \cdot \text{m} \end{aligned}$$

7 C₇H₁₄
methyl-cyclohexane

$$\begin{aligned} T_{c7} &= 572.2 \cdot \text{K} & T_{b7} &= 374.1 \cdot \text{K} & P_{c7} &= 3.47 \cdot 10^6 \cdot \text{Pa} & V_{c7} &= 368 \\ \epsilon_6 &= \frac{T_{c7}}{1.2593} & \sigma_6 &= V_{c7}^{\frac{1}{3}} \cdot 10^{-10} \cdot \text{m} \\ MW_6 &= 98.189 \cdot \text{gm} & \sigma_6 &= 7.1661 \cdot 10^{-10} \cdot \text{m} & \epsilon_6 &= 454.37942 \cdot \text{K} \end{aligned}$$

8 C₉H₁₈
1-nonene

$$\begin{aligned} T_{c9} &= 592 \cdot \text{K} & T_{b9} &= 420 \cdot \text{K} & V_{c9} &= 580 & P_{c9} &= 2.34 \cdot 10^6 \cdot \text{Pa} \\ \epsilon_7 &= \frac{T_{c9}}{1.2593} & \sigma_7 &= V_{c9}^{\frac{1}{3}} \cdot 10^{-10} \cdot \text{m} \\ MW_7 &= 126.243 \cdot \text{gm} & \sigma_7 &= 8.33955 \cdot 10^{-10} \cdot \text{m} & \epsilon_7 &= 470.10244 \cdot \text{K} \end{aligned}$$

9 CO

$$\begin{aligned} \epsilon_8 &= 91.7 \cdot \text{K} & \sigma_8 &= 3.69 \cdot 10^{-10} \cdot \text{m} \\ MW_8 &= 28.01 \cdot \text{gm} \end{aligned}$$

C2
1/38

Define constants for transport integrals:

$$\sigma\mu_{a_0} := 1.16145 \quad \sigma\mu_{b_0} := 0.14874 \quad \sigma Da_0 := 1.06036 \quad \sigma Db_0 := 0.1561$$

$$\sigma\mu_{a_1} := 0.52487 \quad \sigma\mu_{b_1} := 0.7732 \quad \sigma Da_1 := 0.193 \quad \sigma Db_1 := 0.47635$$

$$\sigma\mu_{a_2} := 2.16178 \quad \sigma\mu_{b_2} := 2.43787 \quad \sigma Da_2 := 1.03587 \quad \sigma Db_2 := 1.52996$$

$$\sigma Da_3 := 1.76474 \quad \sigma Db_3 := 3.89411$$

Define transport integrals:

$$\Omega\mu(T) := \sigma\mu_{a_0} \cdot \exp\left[-\left(\sigma\mu_{b_0} \cdot \ln(T)\right)\right] + \sum_{i\mu=1}^2 \sigma\mu_{a_{i\mu}} \cdot \exp\left(-\sigma\mu_{b_{i\mu}} \cdot T\right) \quad \Omega\mu(3) = 1.0394$$

$$\Omega D(T) := \sigma Da_0 \cdot \exp\left[-\left(\sigma Db_0 \cdot \ln(T)\right)\right] + \sum_{i\mu=1}^3 \sigma Da_{i\mu} \cdot \exp\left(-\sigma Db_{i\mu} \cdot T\right) \quad \Omega D(3) = 0.95002$$

Set Inlet Conditions:

$$P := 3 \cdot \text{atm}$$

$$ych40 := 0.01183$$

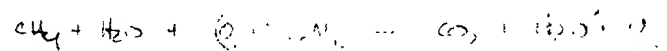
$$y0c5h12 := 0.0028968$$

$$y0c7h14 := 0.0021859$$

$$y0c9h18 := 0.0016878$$

These values for y0i have been determined via enthalpy functions on p. 11 for temperature rise from 1000F to 1511F.

Define gas composition w/r methane using moist (2%) air:



$$y(y0, x) := \begin{bmatrix} y0 \cdot (1 - x) \\ (1 - y0) \cdot 0.205 - 2 \cdot ych40 \cdot x \\ (1 - y0) \cdot 0.775 \\ y0 \cdot x \\ (1 - y0) \cdot 0.02 + 2 \cdot y0 \cdot x \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{matrix} fuel \\ O_2 \\ N_2 \\ CO_2 \\ H_2O \end{matrix}$$

$$y(ych40, 0.1) = \begin{bmatrix} 0.0106 \\ 0.2002 \\ 0.7658 \\ 0.0012 \\ 0.0221 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\sum y(ych40, 0.5) = 1$$

$$(y_{fuel}, x)$$

Define function for calculating stoichiometric gas composition for combustion of 2-methyl-butane using moist (2%) air:

$$C_5H_{12} \quad y5(y0, x) := \frac{\begin{bmatrix} 0 \\ (1-y0) \cdot 0.205 - 8 \cdot y0 \cdot x \\ (1-y0) \cdot 0.775 \\ 5 \cdot (y0 \cdot x) \\ (1-y0) \cdot 0.02 + 6 \cdot y0 \cdot x \\ y0 \cdot (1-x) \\ 0 \\ 0 \end{bmatrix}}{1 + 2 \cdot y0 \cdot x}$$

$\begin{matrix} \text{Fuel} \\ O_2 \\ N_2 \\ CO_2 \\ H_2O \\ C_5H_{12} \end{matrix}$

$$\sum y5(y0c5h12, 0.5) = 1$$

$$y5(y0c5h12, 0.5) = \begin{bmatrix} 0 \\ 0.192262 \\ 0.770523 \\ 0.007221 \\ 0.02855 \\ 0.001444 \\ 0 \\ 0 \end{bmatrix}$$

Define function for calculating stoichiometric gas composition for combustion of methyl-cyclohexane using moist (2%) air:

$$C_7H_{14} \quad y7(y0, x) := \frac{\begin{bmatrix} 0 \\ (1-y0) \cdot 0.205 - 10.5 \cdot y0 \cdot x \\ (1-y0) \cdot 0.775 \\ 7 \cdot (y0 \cdot x) \\ (1-y0) \cdot 0.02 + 7 \cdot y0 \cdot x \\ 0 \\ y0 \cdot (1-x) \\ 0 \end{bmatrix}}{1 + 2.5 \cdot y0 \cdot x}$$

$\begin{matrix} C_7H_{14} \\ C_5H_{12} \\ C_7H_{14} \end{matrix}$

$$\sum y7(y0c7h14, 0.5) = 1$$

$$y7(y0c7h14, 0.5) = \begin{bmatrix} 0 \\ 0.19255 \\ 0.771199 \\ 0.00763 \\ 0.027532 \\ 0 \\ 0.00109 \\ 0 \end{bmatrix}$$

Define function for calculating stoichiometric gas composition for combustion of 1-nonene using moist (2%) air:

$$C_9H_{18} \quad y9(y0, x) := \frac{\begin{bmatrix} 0 \\ (1-y0) \cdot 0.205 - 13.5 \cdot y0 \cdot x \\ (1-y0) \cdot 0.775 \\ 9 \cdot (y0 \cdot x) \\ (1-y0) \cdot 0.02 + 9 \cdot y0 \cdot x \\ 0 \\ 0 \\ y0 \cdot (1-x) \end{bmatrix}}{1 + 3.5 \cdot y0 \cdot x}$$

C_9H_{18}

$$\sum y9(y0c9h18, 0.5) = 1$$

$$y9(y0c9h18, 0.5) = \begin{bmatrix} 0 \\ 0.192692 \\ 0.771413 \\ 0.007573 \\ 0.02748 \\ 0 \\ 0 \\ 8.414148 \cdot 10^{-4} \end{bmatrix}$$

 Define functions for evaluation of mixture properties (ideal gas) given fractional fuel conversion and temperature.

Density and average molecular weight:

$$\rho_{\text{mix}}(x, T) := \left(\sum_{kk=0}^7 y(\text{ych40}, x)_{kk} \cdot \text{MW}_{kk} \right) \cdot \frac{P}{R \cdot T} \quad \text{MW}_{\text{mix}}(x) := \left(\sum_{kk=0}^7 y(\text{ych40}, x)_{kk} \cdot \text{MW}_{kk} \right)$$

$$\rho_{\text{mix}}(1, 300 \cdot \text{K}) = 3.470573 \cdot \text{kg} \cdot \text{m}^{-3}$$

$$\text{MW}_{\text{mix}}(1) = 28.485 \cdot \text{gm}$$

Define diffusion coefficients for specific binary diffusion pairs:

$$\text{Diff}(n, m, T) := 1.8829 \cdot 10^{-27} \cdot \left[\left(\frac{1}{\text{MW}_n} + \frac{1}{\text{MW}_m} \right) \cdot T^3 \right]^{0.5} \cdot 10^8 \cdot \text{gm}^{0.5} \cdot \text{cm}^4 \cdot \text{sec}^{-1} \cdot \text{K}^{-1.5} \cdot \left(\frac{\sigma_n + \sigma_m}{2} \right)^2 \cdot \Omega_D \left[\frac{T}{(\epsilon_n \cdot \epsilon_m)^{0.5}} \right] \cdot \frac{P}{P_{\text{ref}}}$$

$$\text{Diff}(0, 2, 300 \cdot \text{K}) = 0.07417 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\text{Diff}(2, 7, 300 \cdot \text{K}) = 0.01597 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define functions for use with various fuel air mixtures:

$$\text{Dch4}(x, T) := \frac{1 - y(\text{ych40}, x)_0}{\sum_{j\text{gas}=1}^7 \frac{y(\text{ych40}, x)_{j\text{gas}}}{\text{Diff}(0, j\text{gas}, T)}}$$

$$\text{Dch4}(0.5, 298 \cdot \text{K}) = 7.31327 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$\text{Dc5h12}(x, T) := \frac{1 - y5(y0c5h12, x)_0}{\sum_{j\text{gas}=1}^7 \frac{y5(y0c5h12, x)_{j\text{gas}}}{\text{Diff}(5, j\text{gas}, T)}}$$

$$\text{Dc5h12}(0.5, 298 \cdot \text{K}) = 2.28466 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$\text{Dc7h14}(x, T) := \frac{1 - y7(y0c7h14, x)_0}{\sum_{j\text{gas}=1}^7 \frac{y7(y0c7h14, x)_{j\text{gas}}}{\text{Diff}(6, j\text{gas}, T)}}$$

$$\text{Dc7h14}(0.5, 298 \cdot \text{K}) = 1.94254 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

$$\text{Dc9h18}(x, T) := \frac{1 - y9(y0c9h18, x)_0}{\sum_{j\text{gas}=1}^7 \frac{y9(y0c9h18, x)_{j\text{gas}}}{\text{Diff}(7, j\text{gas}, T)}}$$

$$\text{Dc9h18}(0.5, 298 \cdot \text{K}) = 1.53123 \cdot 10^{-6} \cdot \text{m}^2 \cdot \text{sec}^{-1}$$

Display gas mixture properties

$$\text{idsp} := 0..9$$

$$T_{\text{dsp_idsp}} := (750 + 50 \cdot \text{idsp}) \cdot \text{K}$$

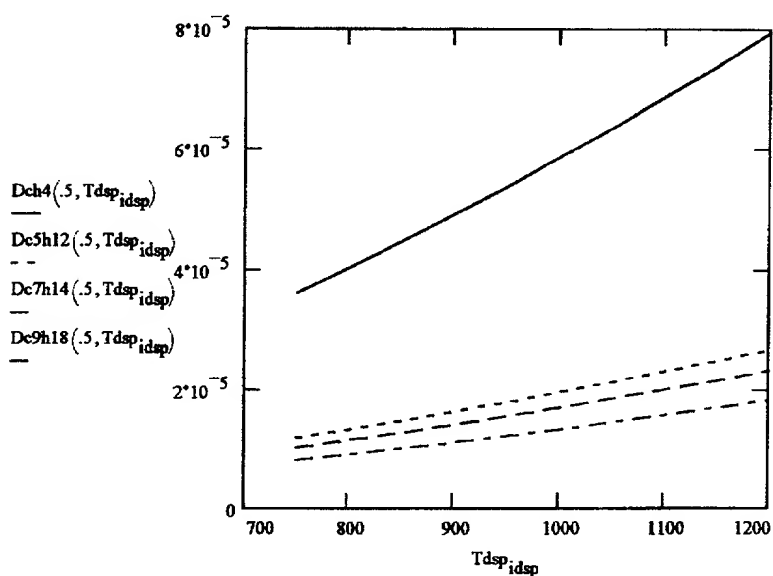
$$T_{\text{in}} := \left[(1000 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K} \quad T_{\text{in}} = 810.92778 \cdot \text{K}$$

$$T_{\text{out}} := \left[(1511 - 32) \cdot \frac{5}{9} + 273.15 \right] \cdot \text{K} \quad T_{\text{out}} = 1094.81667 \cdot \text{K}$$

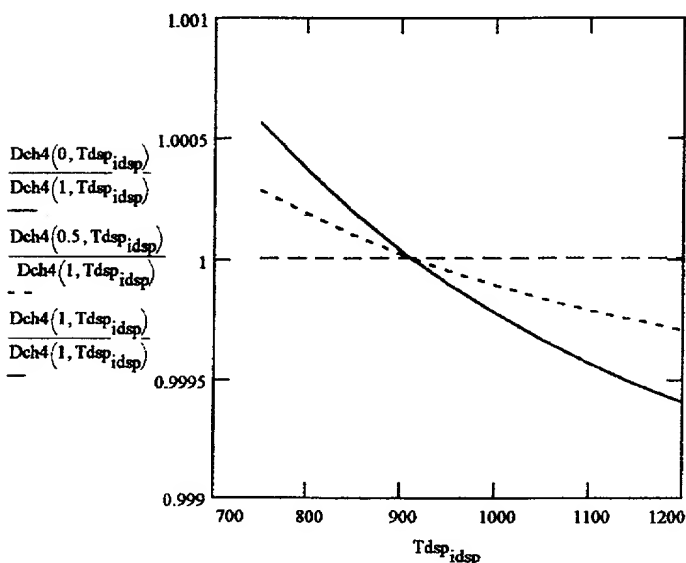
Plots (below) of D_i for CH_4 , C_5H_{12} , etc. show large gap between CH_4 and the other hydrocarbons and show very little effect of fuel conversion (even for methane) on D_i because the fuels are so dilute.

C_7H_{14}

Therefore we can choose methyl cyclohexane as the molecule representative of naphtha and ignore the effect of conversion on gas properties



$T_{\text{dsp_idsp}}$	$D_{\text{ch4}}(.5, T_{\text{dsp_idsp}})$
$7.5 \cdot 10^2 \cdot \text{K}$	$3.61119 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8 \cdot 10^2 \cdot \text{K}$	$4.02644 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8.5 \cdot 10^2 \cdot \text{K}$	$4.45884 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9 \cdot 10^2 \cdot \text{K}$	$4.90801 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9.5 \cdot 10^2 \cdot \text{K}$	$5.37357 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1 \cdot 10^3 \cdot \text{K}$	$5.85522 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.05 \cdot 10^3 \cdot \text{K}$	$6.35265 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.1 \cdot 10^3 \cdot \text{K}$	$6.8656 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.15 \cdot 10^3 \cdot \text{K}$	$7.39384 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.2 \cdot 10^3 \cdot \text{K}$	$7.93712 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$



$T_{\text{dsp_idsp}}$	$D_{\text{c7h14}}(.5, T_{\text{dsp_idsp}})$
$7.5 \cdot 10^2 \cdot \text{K}$	$1.03475 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8 \cdot 10^2 \cdot \text{K}$	$1.15717 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$8.5 \cdot 10^2 \cdot \text{K}$	$1.28482 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9 \cdot 10^2 \cdot \text{K}$	$1.41758 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$9.5 \cdot 10^2 \cdot \text{K}$	$1.55533 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1 \cdot 10^3 \cdot \text{K}$	$1.69798 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.05 \cdot 10^3 \cdot \text{K}$	$1.84541 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.1 \cdot 10^3 \cdot \text{K}$	$1.99755 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.15 \cdot 10^3 \cdot \text{K}$	$2.15429 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.2 \cdot 10^3 \cdot \text{K}$	$2.31555 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$

Define interpolation formulas for Dch4 and Dc7h14 vs. T(K) at x=0.5 via Jandel Scientific's Tablecurve program

$$Dch4T(T) := \exp\left(-11.718527 + 1.6257167 \cdot \ln\left(\frac{T}{K}\right) - \frac{46.77509 \cdot K}{T}\right) \cdot \frac{cm^2}{sec}$$

$$Dch4(.5, 1000 \cdot K) = 0.585522 \cdot sec^{-1} \cdot cm^2$$

$$Dch4T(1000 \cdot K) = 0.585523 \cdot sec^{-1} \cdot cm^2$$

$$Dc7h14T(T) := \exp\left(-12.923061 + 1.6260558 \cdot \ln\left(\frac{T}{K}\right) - \frac{82.480098 \cdot K}{T}\right) \cdot \frac{cm^2}{sec}$$

$$Dc7h14(.5, 1000 \cdot K) = 0.169798 \cdot sec^{-1} \cdot cm$$

$$Dc7h14T(1000 \cdot K) = 0.169798 \cdot sec^{-1} \cdot cm^2$$

Define viscosity functions for major constituents:

$$\mu(T) := \left[\begin{array}{l} \frac{2.6693 \cdot 10^{-26} \cdot (MW_0 \cdot T)^{0.5}}{(\sigma_0)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_0}\right)} \cdot \frac{10^5 \cdot cm}{sec} \cdot \left(\frac{gm}{K}\right)^{0.5} \\ \frac{(MW_1 \cdot T)^{0.5}}{(\sigma_1)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_1}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot cm}{sec}\right) \cdot \left(\frac{gm}{K}\right)^{0.5} \right] \\ \frac{(MW_2 \cdot T)^{0.5}}{(\sigma_2)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_2}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot cm}{sec}\right) \cdot \left(\frac{gm}{K}\right)^{0.5} \right] \\ \frac{(MW_3 \cdot T)^{0.5}}{(\sigma_3)^2 \cdot \Omega \mu \left(\frac{T}{\epsilon_3}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot cm}{sec}\right) \cdot \left(\frac{gm}{K}\right)^{0.5} \right] \\ \frac{1.116 \cdot (MW_4 \cdot T)^{0.5}}{(3.115 \cdot 10^{-8} \cdot cm)^2 \cdot \Omega \mu \left(\frac{T}{514 \cdot K}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\frac{10^5 \cdot cm}{sec}\right) \cdot \left(\frac{gm}{K}\right)^{0.5} \right] \end{array} \right]$$

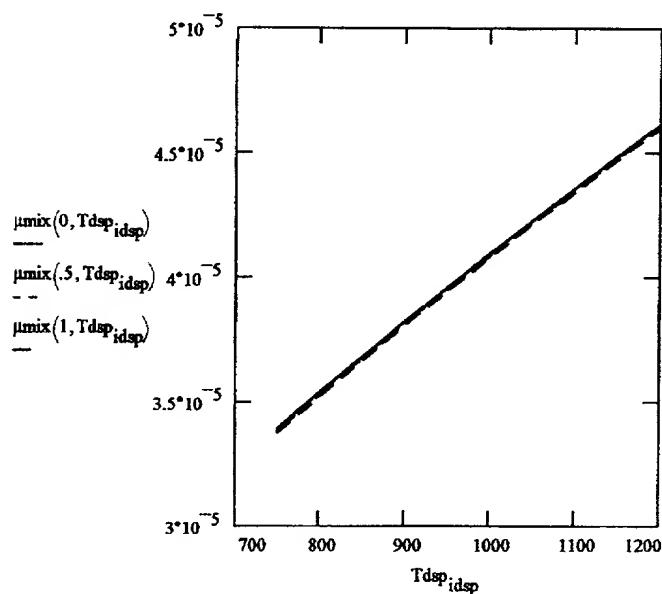
$$\mu(300 \cdot K) = \begin{bmatrix} 1.10281 \cdot 10^{-5} \\ 2.0603 \cdot 10^{-5} \\ 1.76981 \cdot 10^{-5} \\ 1.51851 \cdot 10^{-5} \\ 1.06784 \cdot 10^{-5} \end{bmatrix} \cdot kg \cdot m^{-1} \cdot sec^{-1}$$

$$\mu_{mix}(x, T) := \sum_{n=0}^4 \frac{y(ych40, x)_n \cdot \mu(T)_n}{\sum_{m=0}^4 y(ych40, x)_m \cdot \left[\frac{1 + \left(\frac{\mu(T)_n}{\mu(T)_m}\right)^{0.5} \cdot \left(\frac{MW_m}{MW_n}\right)^{0.25}}{8 \cdot \left(1 + \frac{MW_n}{MW_m}\right)^{0.5}} \right]^2}$$

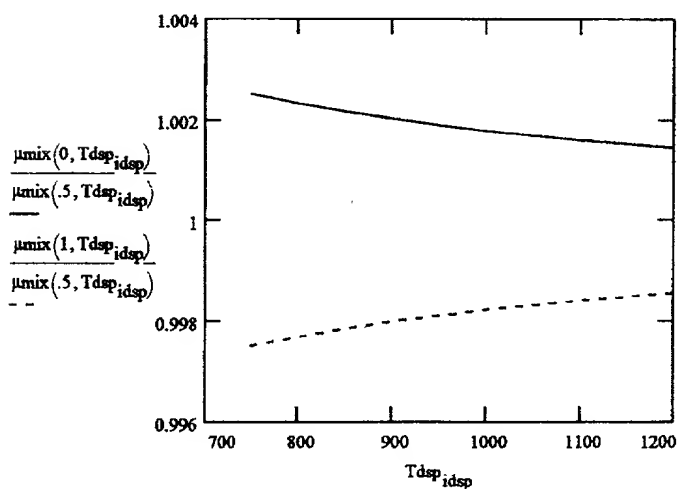
$$y(ych40, 0.5) = \begin{bmatrix} 0.00592 \\ 0.19074 \\ 0.76583 \\ 0.00592 \\ 0.03159 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\mu_{mix}(0.5, 300 \cdot K) = 0.00002 \cdot kg \cdot m^{-1} \cdot sec^{-1}$$

$$ych40 = 0.01183$$



The viscosity of the CH₄ - air mixtures vary little with composition (< 0.5%), again because the fuel is so dilute. We can therefore neglect the effect of composition by choosing $x=0.5$ in all cases.



T_{dsp_idsp}	$\mu_{mix}(0.5, T_{dsp_idsp})$
$7.5 \cdot 10^2 \cdot K$	$3.38338 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$8 \cdot 10^2 \cdot K$	$3.53056 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$8.5 \cdot 10^2 \cdot K$	$3.67429 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$9 \cdot 10^2 \cdot K$	$3.81491 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$9.5 \cdot 10^2 \cdot K$	$3.95267 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$1 \cdot 10^3 \cdot K$	$4.08779 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$1.05 \cdot 10^3 \cdot K$	$4.22047 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$1.1 \cdot 10^3 \cdot K$	$4.35088 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$1.15 \cdot 10^3 \cdot K$	$4.47917 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$
$1.2 \cdot 10^3 \cdot K$	$4.60547 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$

$$\mu_{mix}T(T) := \exp\left(-0.70216045 + 0.640874 \cdot \ln\left(\frac{T}{K}\right) + \frac{-14.24382 \cdot K}{T}\right) \cdot 10^{-6} \cdot kg \cdot m^{-1} \cdot sec^{-1}$$

$$\mu_{mix}(.5, 1000 \cdot K) = 4.08779 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$$

$$\mu_{mix}T(1000 \cdot K) = 4.08782 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$$

Define thermal conductivity functions for light molecules

igas := 0, 1..4

$$a\lambda = \begin{bmatrix} -1.869 \\ -3.273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda = \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda = \begin{bmatrix} 1.179 \cdot 10^{-4} \\ -(3.743 \cdot 10^{-5}) \\ -(5.067 \cdot 10^{-5}) \\ 5.477 \cdot 10^{-6} \\ 1.801 \cdot 10^{-4} \end{bmatrix} \quad d\lambda = \begin{bmatrix} -(3.614 \cdot 10^{-8}) \\ 9.732 \cdot 10^{-9} \\ 1.504 \cdot 10^{-8} \\ -(1.053 \cdot 10^{-8}) \\ -(9.1 \cdot 10^{-8}) \end{bmatrix}$$

CH4
O2
N2
CO2
H2O

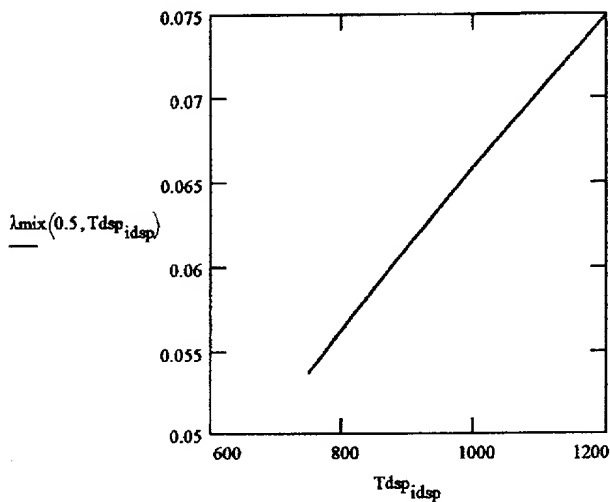
$$\lambda(i, T) := \left[a\lambda_i + b\lambda_i \cdot \frac{T}{K} + c\lambda_i \cdot \left(\frac{T}{K} \right)^2 + d\lambda_i \cdot \left(\frac{T}{K} \right)^3 \right] \cdot 0.00001 \cdot \frac{W}{cm \cdot K}$$

$\lambda(igas, 1000 \cdot K)$ $W/cm/K$

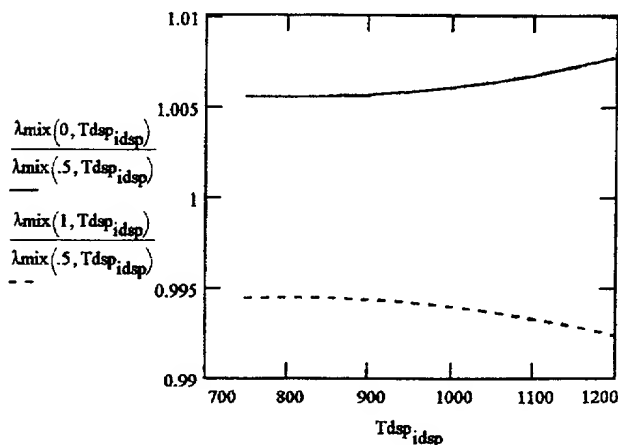
$0.16716 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.07163 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.06292 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.06788 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.08631 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$

$$\lambda_{mix}(x, T) := \frac{\sum_{i=0}^4 y(ych40, x)_i \cdot \lambda(i, T)}{\sum_{j=0}^4 y(ych40, x)_j \cdot \frac{\left[1 + \left(\frac{\mu(T)_i}{\mu(T)_j} \right)^{0.5} \cdot \left(\frac{MW_j}{MW_i} \right)^{0.25} \right]^2}{\left[8 \cdot \left(1 + \frac{MW_i}{MW_j} \right) \right]^{0.5}}}$$

$$\lambda_{mix}(0, 1000 \cdot K) = 0.00066 \cdot \frac{W}{cm \cdot K}$$



$Tdsp_{idsp}$	$\lambda_{mix}(0.5, Tdsp_{idsp})$
$7.5 \cdot 10^2 \cdot K$	$0.05362 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$8 \cdot 10^2 \cdot K$	$0.05621 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$8.5 \cdot 10^2 \cdot K$	$0.05872 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$9 \cdot 10^2 \cdot K$	$0.06117 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$9.5 \cdot 10^2 \cdot K$	$0.06355 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1 \cdot 10^3 \cdot K$	$0.06589 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.05 \cdot 10^3 \cdot K$	$0.06818 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.1 \cdot 10^3 \cdot K$	$0.07043 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.15 \cdot 10^3 \cdot K$	$0.07266 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.2 \cdot 10^3 \cdot K$	$0.07488 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$



The thermal conductivity varies > 1% with conversion. Selection of 50% conversion gives an error range of +.5-.5% at 1000K. This is likely to be smaller than the accuracy of measured thermal conductivity. Therefore we again define a composition independent formula to increase speed in calculating derived transport properties

$$\lambda_{\text{mix}}(T) := \exp\left(-7.073383 + 0.6397005 \cdot \ln\left(\frac{T}{K}\right) + \frac{-65.2387 \cdot K}{T}\right) \cdot W \cdot m^{-1} \cdot K^{-1}$$

$$\lambda_{\text{mix}}(.5, 1000 \cdot K) = 0.06589 \cdot m^{-1} \cdot K^{-1} \cdot W$$

$$\lambda_{\text{mix}}(1000 \cdot K) = 0.06589 \cdot m^{-1} \cdot K^{-1} \cdot W$$

Determine the heat capacity and enthalpy functions of the fuel-air mixtures for the evaluation of temperature rise

Define heat capacities and heat of combustion:

$$Cp_{\text{coef}} := \begin{bmatrix} 19.25 & .05213 & 0.00001197 & -0.00000001132 \\ 28.11 & -0.000368 & 0.00001746 & -0.00000001065 \\ 31.15 & -0.01357 & 0.0000268 & -0.00000001168 \\ 19.8 & 0.07344 & -0.00005602 & 0.00000001715 \\ 32.24 & 0.001924 & 0.00001055 & -0.000000003596 \\ -9.52 & 0.5066 & -0.0002729 & 0.00000005723 \\ -76.19 & 0.7867 & -0.0004204 & 0.00000007516 \\ -37.18 & 0.8122 & -0.0004509 & 0.00000009705 \end{bmatrix}$$

$$Cp(\text{igas}, T) := \sum_{jj=0}^3 Cp_{\text{coef}}_{\text{igas}, jj} \left(\frac{T}{K}\right)^{jj} \cdot \frac{J}{K}$$

J/mol/K

$$Cp(0, 300 \cdot K) = 35.66066 \cdot K^{-1} \cdot J$$

$$Cp(5, 300 \cdot K) = 119.44421 \cdot K^{-1} \cdot J$$

$$Cp(6, 300 \cdot K) = 124.01332 \cdot K^{-1} \cdot J$$

$$Cp(7, 300 \cdot K) = 168.51935 \cdot K^{-1} \cdot J$$

$$Cp_{\text{mix}}(x, T) := \sum_{jk=0}^4 Cp(jk, T) \cdot y(\text{ych40}, x)_{jk}$$

$$Cp_{\text{mix}}(0.5, 998 \cdot K) = 33.66993 \cdot J \cdot K^{-1}$$

$$y(\text{ych40}, 0.5) = \begin{bmatrix} 0.00592 \\ 0.19074 \\ 0.76583 \\ 0.00592 \\ 0.03159 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

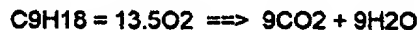
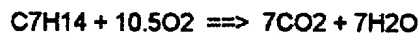
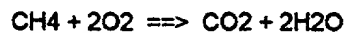
Define heats of combustion

$$\Delta C_{pcomb}(T) := (C_p(3, T) + 2 \cdot C_p(4, T)) - (C_p(0, T) + 2 \cdot C_p(1, T))$$

$$\Delta C_{pcomb5}(T) := (5 \cdot C_p(3, T) + 6 \cdot C_p(4, T)) - (C_p(5, T) + 8 \cdot C_p(1, T))$$

$$\Delta C_{pcomb7}(T) := (7 \cdot C_p(3, T) + 7 \cdot C_p(4, T)) - (C_p(6, T) + 10.5 \cdot C_p(1, T))$$

$$\Delta C_{pcomb9}(T) := (9 \cdot C_p(3, T) + 9 \cdot C_p(4, T)) - (C_p(7, T) + 13.5 \cdot C_p(1, T))$$



$$\Delta H_f := \begin{bmatrix} -74900 \cdot J \\ 0 \cdot J \\ 0 \cdot J \\ -393800 \cdot J \\ -242000 \cdot J \\ -154600 \cdot J \\ -119400 \cdot J \\ -103600 \cdot J \end{bmatrix}$$

$$\Delta C_{pcomb}(298 \cdot K) = 10.38812 \cdot K^{-1} \cdot J$$

$$\frac{\Delta C_{pcomb7}(298 \cdot K)}{7} = 9.35823 \cdot K^{-1} \cdot J$$

$$\frac{\Delta C_{pcomb5}(298 \cdot K)}{5} = 6.97449 \cdot kg \cdot m^2 \cdot sec^{-2} \cdot K^{-1}$$

$$\frac{\Delta C_{pcomb9}(298 \cdot K)}{9} = 8.3177 \cdot K^{-1} \cdot J$$

Define enthalpy function for individual components and ΔH for fuels:

$$H_f(nn, T) := \Delta H_{f_m} + \int_{298 \cdot K}^T C_p(nn, T_x) dT_x$$

$$\Delta H_{comb}(T) := \left[(\Delta H_{f_3} + 2 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 2 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb}(T_x) dT_x$$

$$\Delta H_{comb5}(T) := \left[(5 \cdot \Delta H_{f_3} + 6 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 8 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb5}(T_x) dT_x$$

$$\Delta H_{comb7}(T) := \left[(7 \cdot \Delta H_{f_3} + 7 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 10.5 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb7}(T_x) dT_x$$

$$\Delta H_{comb9}(T) := \left[(9 \cdot \Delta H_{f_3} + 9 \cdot \Delta H_{f_4}) - (\Delta H_{f_0} + 13.5 \cdot \Delta H_{f_1}) \right] + \int_{298 \cdot K}^T \Delta C_{pcomb9}(T_x) dT_x$$

Hf(igas, 1000·K)

-36559.44819·kg·m ² ·sec ⁻²
22590.03871·kg·m ² ·sec ⁻²
21484.78794·kg·m ² ·sec ⁻²
-3.60367·10 ⁵ ·kg·m ² ·sec ⁻²
-2.15959·10 ⁵ ·kg·m ² ·sec ⁻²

Evaluate a few values of ΔH for CH₄, C₅H₁₂, C₇H₁₄, and C₉H₁₈:

$$\Delta H_{comb}(800 \cdot K) = -8.00306 \cdot 10^5 \cdot J \quad \frac{\Delta H_{comb5}(800 \cdot K)}{5} = -6.69221 \cdot 10^5 \cdot J$$

$$\frac{\Delta H_{comb7}(800 \cdot K)}{7} = -6.2472 \cdot 10^5 \cdot J \quad \frac{\Delta H_{comb9}(800 \cdot K)}{9} = -6.26002 \cdot 10^5 \cdot J$$

Define the mixture enthalpies and determine the fuel composition needed for 511F temperature rise from 1000F.

igas := 0, 1..7

$$H_{mix}(x, T) := \sum_{k_{gas}=0}^7 y(y_{ch40}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{ch40} = 0.01183$$

$$H_{mix}(0, 810.93 \cdot K) = 1.006514 \cdot 10^4 \cdot J \quad H_{mix}(1, 1094.82 \cdot K) = 1.006518 \cdot 10^4 \cdot J$$

Determines CH4 inlet concentration

$$H_{mix5}(x, T) := \sum_{k_{gas}=0}^7 y5(y_{0c5h12}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{0c5h12} = 0.0028968$$

$$H_{mix5}(0, 810.93 \cdot K) = 1.058499 \cdot 10^4 \cdot J \quad H_{mix5}(1, 1094.82 \cdot K) = 1.058492 \cdot 10^4 \cdot J$$

Determines C5H12 inlet concentration

$$H_{mix7}(x, T) := \sum_{k_{gas}=0}^7 y7(y_{0c7h14}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{0c7h14} = 0.0021859$$

$$H_{mix7}(0, 810.93 \cdot K) = 1.075807 \cdot 10^4 \cdot J \quad H_{mix7}(1, 1094.82 \cdot K) = 1.075812 \cdot 10^4 \cdot J$$

Determines C7H14 inlet concentration

$$H_{mix9}(x, T) := \sum_{k_{gas}=0}^7 y9(y_{0c9h18}, x)_{k_{gas}} \cdot H_f(k_{gas}, T) \quad y_{0c9h18} = 0.0016878$$

$$H_{mix9}(0, 810.93 \cdot K) = 1.083024 \cdot 10^4 \cdot J \quad H_{mix9}(1, 1094.82 \cdot K) = 1.083028 \cdot 10^4 \cdot J$$

Determines C9H18 inlet concentration

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Define momentum and thermal diffusivities:

$$P = 3.039 \cdot 10^5 \cdot \text{Pa}$$

$$\alpha(\text{igas}, T) := \frac{\lambda(\text{igas}, T) \cdot R \cdot T}{Cp(\text{igas}, T) \cdot P}$$

$$\alpha(0, 300\text{K}) = 0.07813 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$\alpha_{\text{mix}}(x, T) := \frac{\lambda_{\text{mix}}(x, T) \cdot R \cdot T}{Cp_{\text{mix}}(x, T) \cdot P}$$

$$\alpha_{\text{mix}}(.5, 1000\text{K}) = 0.5352 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$v_{\text{mix}}(x, T) := \frac{\mu_{\text{mix}}(x, T)}{\rho_{\text{mix}}(x, T)}$$

$$\rho_{\text{mix}}(.5, 1000\text{K}) = 1.04117 \cdot 10^{-3} \cdot \text{gm} \cdot \text{cm}^{-3}$$

$$v_{\text{mix}}(.5, 1000\text{K}) = 0.3926 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{ch4}}(.5, 1000\text{K}) = 0.5855 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c5h12}}(.5, 1000\text{K}) = 0.1957 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c7h14}}(0.5, 1000\text{K}) = 0.1698 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{c9h18}}(.5, 1000\text{K}) = 0.13431 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

Define Prandtl, Schmidt, and Lewis numbers

$$Pr(x, T) := \frac{v_{\text{mix}}(x, T)}{\alpha_{\text{mix}}(x, T)}$$

$$Pr(.5, 1000\text{K}) = 0.73359$$

$$Sc(x, T) := \frac{v_{\text{mix}}(x, T)}{D_{\text{ch4}}(x, T)}$$

$$Sc(.5, 1000\text{K}) = 0.67054$$

$$Sc_5(x, T) := \frac{v_{\text{mix}}(x, T)}{D_{\text{c5h12}}(x, T)}$$

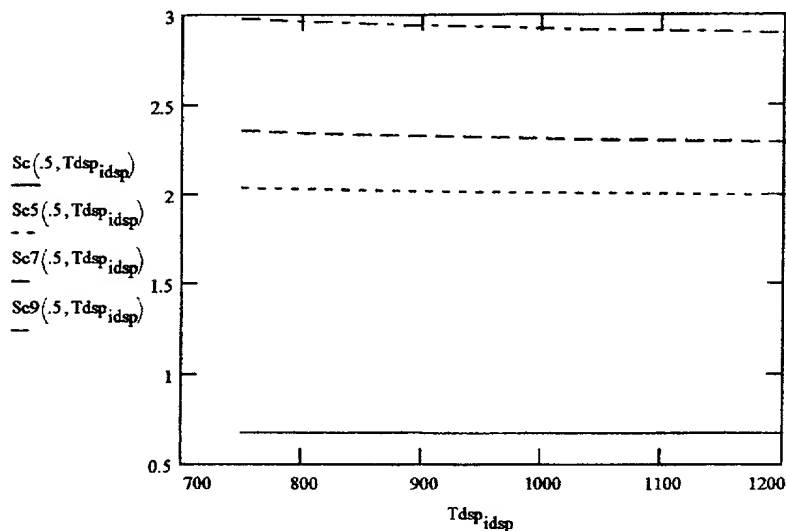
$$Sc_5(.5, 1000\text{K}) = 2.00639$$

$$Sc_7(x, T) := \frac{v_{\text{mix}}(x, T)}{D_{\text{c7h14}}(x, T)}$$

$$Sc_7(.5, 1000\text{K}) = 2.31224$$

$$Sc_9(x, T) := \frac{v_{\text{mix}}(x, T)}{D_{\text{c9h18}}(x, T)}$$

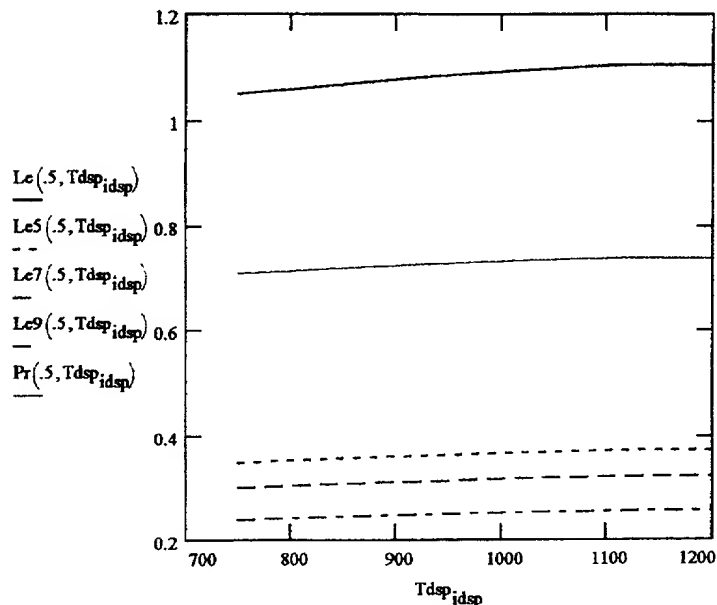
$$Sc_9(.5, 1000\text{K}) = 2.92325$$



These relations have weak temperature dependence and (presumably) very weak dependence on composition

$$Le(x, T) := \frac{D_{ch4}(x, T)}{\alpha_{mix}(x, T)} \quad Le(.5, 1000 \cdot K) = 1.09404 \quad Le5(x, T) := \frac{D_{c5h12}(x, T)}{\alpha_{mix}(x, T)} \quad Le5(.5, 1000 \cdot K) = 0.36563$$

$$Le7(x, T) := \frac{D_{c7h14}(x, T)}{\alpha_{mix}(x, T)} \quad Le7(.5, 1000 \cdot K) = 0.31726 \quad Le9(x, T) := \frac{D_{c9h18}(x, T)}{\alpha_{mix}(x, T)} \quad Le9(.5, 1000 \cdot K) = 0.25095$$



The Lewis numbers show approximately the temperature rise at the wall of an active catalyst relative to the adiabatic temperature rise at that point.

Clearly temperature (and composition) have little influence on the ΔT at the wall, while the nature of the fuel molecule has a strong effect (from $0.25 \cdot \Delta T_{adiab}$ for C9 to $1.1 \cdot \Delta T_{adiab}$ for CH4)

Can remove compositional dependence for most property functions

$$\rho_{mixT}(T) := MW_{mix}(0.5) \cdot \frac{P}{R \cdot T}$$

$$v_{mixT}(T) = \frac{\mu_{mixT}(T)}{\rho_{mixT}(T)}$$

$$ScT(T) := \frac{\mu_{mixT}(T)}{D_{ch4T}(T) \cdot \rho_{mix}(0.5, T)}$$

$$Sc7T(T) := \frac{\mu_{mixT}(T)}{D_{c7h14T}(T) \cdot \rho_{mix}(0.5, T)}$$

These functions speed calculations of Nu numbers and heat and mass transfer coefficients

This ends the extended section that defines gas properties for the combustion of several fuel air mixtures.

Define honeycomb configurations

$$\text{Diao} := 9\text{-in} \quad \text{Diao} = 22.86 \cdot \text{cm} \quad \text{Diai} := 4\text{-in} \quad \text{Diai} = 10.16 \cdot \text{cm} \quad \text{Lhc} := 3.5\text{-in} \quad \text{Lhc} = 8.89 \cdot \text{cm}$$

With bypass change Diao to 8.5 in Bypass := 0 Bypass = 0, 0.2, 0.4 Lhc = 3.5, 4 in

Honeycombs: Represent as square channel metal alloy wall 0.05 mm, uncoated

$$\text{Cells1} := 100 \cdot \text{in}^{-2} \quad \text{dwall1} := 0.009 \cdot \text{cm} \quad \text{Cells2} := 200 \cdot \text{in}^{-2} \quad \text{dwall2} := 0.009 \cdot \text{cm}$$

$$\text{dcell1} := (\text{Cells1})^{-0.5} - \text{dwall1} \quad \text{dcell2} := (\text{Cells2})^{-0.5} - \text{dwall2}$$

$$\text{dcell1} = 0.245 \cdot \text{cm} \quad \text{ks1} := 0.002 \cdot \text{cm} \quad \text{dcell2} = 0.17061 \cdot \text{cm} \quad \text{ks2} := 0.002 \cdot \text{cm}$$

$$\text{scell1} := \text{dcell1}^2 \cdot \text{Cells1} \quad \text{scell1} = 0.93039 \quad \text{scell2} := \text{dcell2}^2 \cdot \text{Cells2} \quad \text{scell2} = 0.90229$$

$$\text{Cells4} := 400 \cdot \text{in}^{-2} \quad \text{dwall4} := 0.007 \cdot \text{cm}$$

$$\text{Cells6} := 600 \cdot \text{in}^{-2} \quad \text{dwall6} := 0.007 \cdot \text{cm}$$

$$\text{dcell4} := (\text{Cells4})^{-0.5} - \text{dwall4} \quad \text{dcell4} = 0.12 \cdot \text{cm}$$

$$\text{dcell6} := (\text{Cells6})^{-0.5} - \text{dwall6} \quad \text{dcell6} = 0.0967 \cdot \text{cm}$$

$$\text{dcell4} = 0.12 \cdot \text{cm} \quad \text{ks4} := 0.001 \cdot \text{cm}$$

$$\text{dcell6} = 0.0967 \cdot \text{cm} \quad \text{ks6} := 0.001 \cdot \text{cm}$$

$$\text{scell4} := \text{dcell4}^2 \cdot \text{Cells4} \quad \text{scell4} = 0.8928$$

$$\text{scell6} := \text{dcell6}^2 \cdot \text{Cells6} \quad \text{scell6} = 0.86955$$

Describe 100 and 200 cpi dimensions, although not expected to be used

Packed Beds: Cylindrical (conical) geometry

$$\text{Dinr} := 6\text{-in}$$

$$\text{Doutr} := 7\text{-in}$$

$$\text{Wbed} := 7\text{-in}$$

$$\text{Lbed} := 0.75\text{-in}$$

$$\text{Dinr} = 15.24 \cdot \text{cm}$$

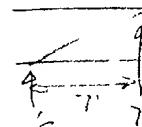
$$\text{Doutr} = 17.78 \cdot \text{cm}$$

$$\text{Wbed} = 17.78 \cdot \text{cm}$$

$$\text{Smono} := \frac{\pi}{4} (\text{Diao}^2 - \text{Diai}^2)$$

$$\text{Sbed} := \pi \cdot \left(\frac{\text{Dinr} + \text{Doutr}}{2} \right) \cdot \text{Wbed}$$

$$\frac{\text{Smono}}{\text{Sbed}} = 0.35714$$



Define initial combustion conditions

Adjust U0 to fit U(Tin)=7 m/sec w/o bypass flow

$$\text{Uref} := 7 \cdot \frac{\text{m}}{\text{sec}}$$

$$\text{Tin} := (537.778 + 273.15) \cdot \text{K}$$

$$\text{Tin} = 810.928 \cdot \text{K}$$

$$\text{P} = 3.039 \cdot 10^5 \cdot \text{kg} \cdot \text{m}^{-1} \cdot \text{sec}^{-2}$$

$$\text{M0} := \text{Uref} \cdot \rho_{\text{mix}}(0, \text{Tin}) \cdot \left[\frac{\pi}{4} ((9\text{-in})^2 - (4\text{-in})^2) \right]$$

$$\text{M0} = 0.29601 \cdot \text{kg} \cdot \text{sec}^{-1}$$

$$\text{Tout} := (821.667 + 273.15) \cdot \text{K}$$

$$\text{U0} := \frac{\text{M0} \cdot (1 - \text{Bypass})}{\rho_{\text{mix}}(0, \text{Tin}) \cdot \frac{\pi}{4} (\text{Diao}^2 - \text{Diai}^2)}$$

$$\text{Tout} = 1094.817 \cdot \text{K}$$

$$\text{U(T)} := \text{U0} \cdot \frac{\text{T}}{\text{Tin}}$$

$$\text{U(Tin)} = 7 \cdot \text{m} \cdot \text{sec}^{-1}$$

$$\text{G0} = \text{U(Tin)} \cdot \rho_{\text{mix}}(0, \text{Tin})$$

$$\text{Ubed(T)} := \frac{\text{M0}}{\rho_{\text{mix}}(0, \text{Tin}) \cdot \text{Sbed}}$$

$$\text{Ubed(Tin)} = 2.5 \cdot \text{m} \cdot \text{sec}^{-1}$$

$$\text{G0} = 8.98749 \cdot \text{kg} \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$\text{Rehc4}(T) := \frac{G0 \cdot d_{\text{cell4}}}{s_{\text{cell4}} \cdot \mu_{\text{mix}}(T)} \quad \text{Rehc4}(T_{\text{in}}) = 339.11451$$

$$\text{Rehc6}(T) := \frac{G0 \cdot d_{\text{cell6}}}{s_{\text{cell6}} \cdot \mu_{\text{mix}}(T)} \quad \text{Rehc6}(T_{\text{in}}) = 280.56407$$

For laminar flow with entrance effect (adapted from Kays & Crawford, "Convective Heat and Mass Transfer"):

$$\text{cfric4}(T, z) := \frac{14.227}{\text{Rehc4}(T)} \left[1 + 0.046263 \cdot \left(\text{Rehc4}(T) \cdot \frac{d_{\text{cell4}}}{z} \right) \right]^{0.45363}$$

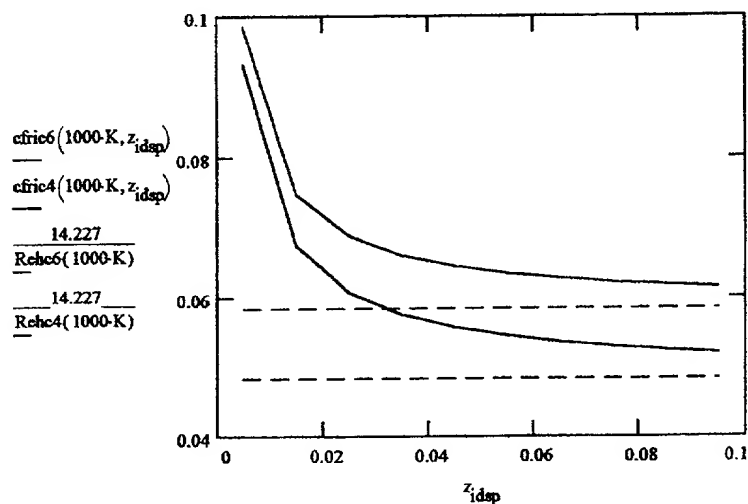
$$\text{cfric6}(T, z) := \frac{14.227}{\text{Rehc6}(T)} \left[1 + 0.046263 \cdot \left(\text{Rehc6}(T) \cdot \frac{d_{\text{cell6}}}{z} \right) \right]^{0.45363}$$

Average coefficient of friction

Calculate monolith pressure drop in several monoliths with entrance effect:

$$z_{\text{idsp}} := 0.5 \cdot \text{cm} + 1 \cdot \text{idsp} \cdot \text{cm}$$

$$U_{\text{dsp}} = (4 + \text{idsp}) \cdot \text{m} \cdot \text{sec}^{-1}$$



The entrance effect for ΔP of a channel in laminar flow is significant even to 3.5 in. length.

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$$T_{avg} := \frac{T_{in} + T_{out}}{2}$$

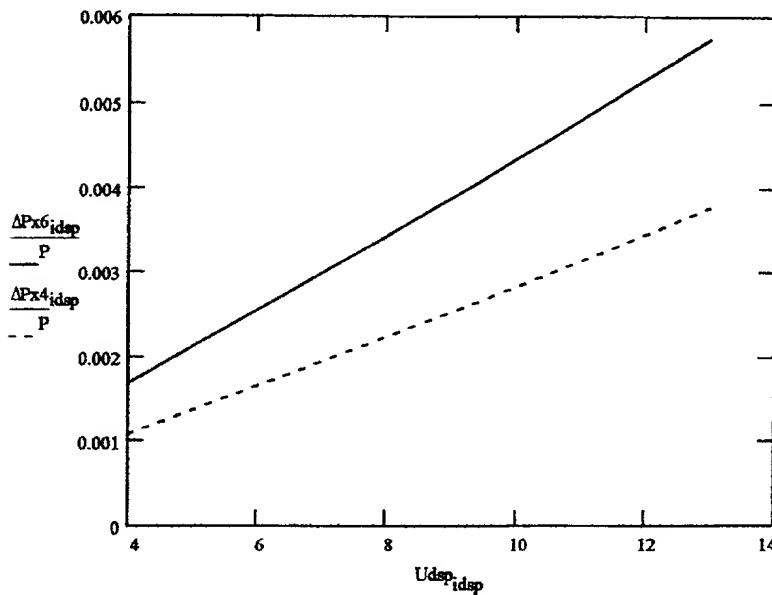
$$c_{f,icx}(x,z) = \frac{14.227}{x} \cdot (1 + 0.0462363 \cdot (x \cdot z))^{0.45363}$$

$$Re_{x6}_{idsp} := \frac{d_{cell6}}{s_{cell6}} \cdot \frac{U_{dsp}_{idsp}}{v_{mix}T(T_{avg})}$$

$$Re_{x4}_{idsp} := \frac{d_{cell4}}{s_{cell4}} \cdot \frac{U_{dsp}_{idsp}}{v_{mix}T(T_{avg})}$$

$$\Delta P_{x4}_{idsp} := 4 \cdot c_{f,icx}\left(Re_{x4}_{idsp}, \frac{d_{cell4}}{L_{hc}}\right) \cdot \frac{\rho_{mix}T(T_{avg})}{2} \cdot \left(\frac{U_{dsp}_{idsp}}{s_{cell4}}\right)^2 \cdot \frac{L_{hc}}{d_{cell4}}$$

$$\Delta P_{x6}_{idsp} := 4 \cdot c_{f,icx}\left(Re_{x6}_{idsp}, \frac{d_{cell6}}{L_{hc}}\right) \cdot \frac{\rho_{mix}T(T_{avg})}{2} \cdot \left(\frac{U_{dsp}_{idsp}}{s_{cell6}}\right)^2 \cdot \frac{L_{hc}}{d_{cell6}}$$



$\Delta P/P < 0.5\%$ to about 11 m/sec

$$\Delta Phc6(T) := 4 \cdot c_{f,ic6}(T, L_{hc}) \cdot \frac{\rho_{mix}T(T) \cdot \left(\frac{U(T)}{s_{cell6}}\right)^2}{2} \cdot \frac{L_{hc}}{d_{cell6}}$$

$$T_{avg} = 952.8725 \cdot K$$

$$U(T_{avg}) = 8.22528 \cdot m \cdot sec^{-1}$$

$$\frac{\Delta Phc6(T_{in})}{P} = 0.00271$$

$$\frac{\Delta Phc6(T_{out})}{P} = 0.00441$$

$$\frac{\Delta Phc6(T_{avg})}{P} = 0.00352$$

$$\Delta Phc4(T) := 4 \cdot c_{f,ic4}(T, L_{hc}) \cdot \frac{\rho_{mix}T(T) \cdot \left(\frac{U(T)}{s_{cell4}}\right)^2}{2} \cdot \frac{L_{hc}}{d_{cell4}}$$

$$\frac{\Delta Phc4(T_{avg})}{P} = 0.00228$$

Find 1-D heat and mass transfer rates via Nusselt formulas

Averaged Nu for 600 cpi square channels (fully developed laminar flow) taken from Rosner:

$$\text{NuhavgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$\frac{7.6 \cdot (2 \cdot \text{cm})}{\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dccl6}} = 0.85369$$

$$\text{NuhavgR6}(\text{Lhc}) = 2.98649$$

$$\text{NumavgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{ScT}(\text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$\text{NumavgR6}(\text{Lhc}) = 2.98441$$

$$\text{Num5avgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc5}(.5, \text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$\text{Num5avgR6}(\text{Lhc}) = 3.11102$$

$$\text{Num7avgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$\text{Num7avgR6}(\text{Lhc}) = 3.16167$$

$$\text{Num7avgR4}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc4}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dccl4}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$\text{Num7avgR4}(\text{Lhc}) = 3.3902$$

$$\text{Num9avgR6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc9}(.5, \text{Tavg}) \cdot \text{dccl6}} \right)^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$\text{Num9avgR6}(\text{Lhc}) = 3.2775$$

The Nusselt numbers for mass transfer show small (< 5%) compensation for the low diffusivity of the higher hydrocarbons.

Use exponential functions implied by the definition of average (integrated) Num functions to calculate exit mole fractions.

$$y_{c7h14}(T, z) = y_{0c7h14} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Num7avgR6}(z)}{\text{Rehc6}(T) \cdot \text{Sc7T}(T) \cdot \text{dcell6}}\right)$$

$$\frac{y_{c7h14}(\text{Tavg}, \text{Lhc})}{y_{0c7h14}} = 0.13705$$

$$y_{ch4}(T, z) = y_{ch40} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{NumavgR6}(z)}{\text{Rehc6}(T) \cdot \text{ScT}(T) \cdot \text{dcell6}}\right)$$

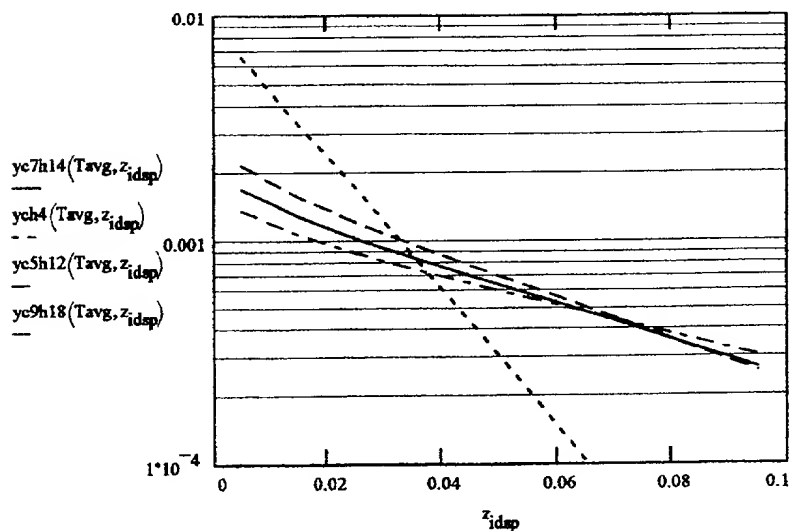
$$\frac{y_{ch4}(\text{Tavg}, \text{Lhc})}{y_{ch40}} = 0.001533$$

$$y_{c5h12}(T, z) = y_{0c5h12} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Num7avgR6}(z)}{\text{Rehc6}(T) \cdot \text{Sc5}(0.5, T) \cdot \text{dcell6}}\right)$$

$$\frac{y_{c5h12}(\text{Tavg}, \text{Lhc})}{y_{0c5h12}} = 0.10114$$

$$y_{c9h18}(T, z) = y_{0c9h18} \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Num9avgR6}(z)}{\text{Rehc6}(T) \cdot \text{Sc9}(0.5, T) \cdot \text{dcell6}}\right)$$

$$\frac{y_{c9h18}(\text{Tavg}, \text{Lhc})}{y_{0c9h18}} = 0.19604$$



$$z_g = 0.095 \cdot \text{m}$$

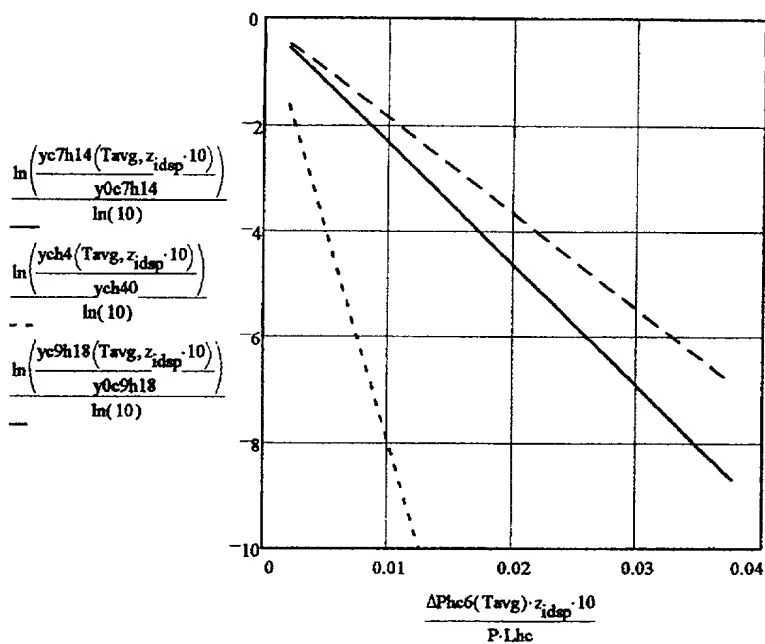
$$z_g = 3.74016 \cdot \text{in}$$

Summary if 600 cpi Metal Monolith Performance

%Bypass	Length(in)	Diao(in)	Yout/Yin C7H14	Yout/Yin CH4	ΔP/P
0	3.5	9.0	0.13705	0.001533	0.00352
0	4	9.0	0.10679	0.000611	0.00400
20	3.5	8.5	0.11888	0.000906	0.00324
20	4	8.5	0.09055	0.000335	0.00368
40	3.5	8.5	0.06266	0.000089	0.00240
40	4	8.5	0.04317	0.000023	0.00273

Bypass = 0
Lhc = 3.5 in
Diao = 9 in

These values are conservative and do not account for the higher average temperature with the higher F/A ratios and do not account for hydrothermal entry.



Constant Flow 8.2 m/sec
Variable Length to 89 cm

$$U(T_{avg}) = 8.22528 \cdot m \cdot sec^{-1}$$

$$10 \cdot L_{hc} = 88.9 \cdot cm$$

Conversions at $\Delta P/P = 0.01$

$$CH_4 = 1.06 \cdot 10^{-8}$$

$$C_7H_{14} = 4.8 \cdot 10^{-3}$$

$$C_9H_{18} = 1.44 \cdot 10^{-2}$$

$$z = 25.25 \cdot cm$$

$$z_x = 25.25 \cdot cm$$

$$\frac{\Delta Phc6(T_{avg}) \cdot z_x}{P \cdot L_{hc}} = 0.01000$$

$$\frac{yc7h14(T_{avg}, z_x)}{y0c7h14} = 4.80371 \cdot 10^{-3}$$

$$\frac{ych4(T_{avg}, z_x)}{ych40} = 1.06492 \cdot 10^{-8}$$

$$\frac{yc9h18(T_{avg}, z_x)}{y0c9h18} = 1.44218 \cdot 10^{-2}$$

Conversions at $\Delta P/P = 0.02$

$$CH_4 = 1.14 \cdot 10^{-16}$$

$$C_7H_{14} = 2.41 \cdot 10^{-5}$$

$$C_9H_{18} = 2.21 \cdot 10^{-4}$$

$$z = 50.5 \cdot cm$$

The 600 cpi monolith has low pressure drop at 8.89 cm length. If it's length were extended to give 1.0% and 2.0% fractional pressure drop, then C_7H_{14} conversions would increase to 99.5% and 99.998% respectively

Set up properties for CO to calculate the conversion of dilute CO and hydrocarbons downstream of the turbine

$$D_{co1}(x, T) := \frac{\frac{P}{Pref}}{\sum_{jgas=0}^7 \frac{y(ych40, x)_{jgas}}{Diff(8, jgas, T)}}$$

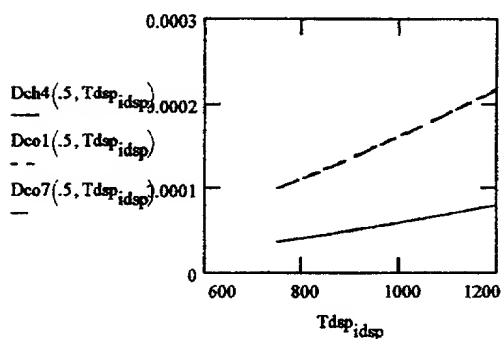
$$D_{co1}(.5, T_{in}) = 1.12854 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad Pref = 1 \cdot \text{atm}$$

$$D_{ch4}(.5, T_{in}) = 0.41195 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad P = 3 \cdot \text{atm}$$

$$D_{co7}(x, T) := \frac{\frac{P}{Pref}}{\sum_{jgas=0}^7 \frac{y7(y0c7h14, x)_{jgas}}{Diff(8, jgas, T)}}$$

$$D_{co7}(.5, T_{in}) = 1.12396 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad Pref = 1 \cdot \text{atm}$$

$$D_{c7h14}(.5, T_{in}) = 0.11846 \cdot \text{sec}^{-1} \cdot \text{cm}^2 \quad P = 3 \cdot \text{atm}$$



T_{dsp_idsp}

750-K
800-K
850-K
900-K
950-K
1000-K
1050-K
1100-K
1150-K
1200-K

$D_{co1}(.5, T_{dsp_idsp})$

$9.90331 \cdot 10^{-5} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.10324 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.2208 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.34291 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.46949 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.60044 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.73572 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$1.87523 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$2.01893 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$
$2.16675 \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1}$

$$D_{coT}(T) := \exp \left[\left(-10.80086 + 1.6357427 \cdot \ln \left(\frac{T}{K} \right) - 28.157906 \cdot \frac{K}{T} \right) \cdot 10^{-4} \cdot \text{m}^2 \cdot \text{sec}^{-1} \right]$$

$$D_{co1}(.5, T_{avg}) = 1.47689 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{coT}(T_{avg}) = 1.47689 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$d_{reco} := 17 \cdot \text{in}$$

$$d_{reco} = 43.18 \cdot \text{cm}$$

$$L_{rec} = 3.5 \cdot \text{in}$$

$$d_{reci} := 6 \cdot \text{in}$$

$$d_{reci} = 15.24 \cdot \text{cm}$$

$$L_{rec} = 8.89 \cdot \text{cm}$$

$$M0 = 0.29601 \cdot \text{kg} \cdot \text{sec}^{-1}$$

$$A_{recup} = \pi \cdot \frac{d_{reco}^2 - d_{reci}^2}{4}$$

$$A_{recup} = 0.1282 \cdot \text{m}^2$$

$$G_{rec0} := \frac{M0}{A_{recup}}$$

$$G_{rec0} = 2.30904 \cdot \text{kg} \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

$$G0 = 8.98749 \cdot \text{kg} \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

$$P_{rec} := 1 \cdot \text{atm}$$

$$\rho_{mixrec}(T) = \frac{MW_{mix}(0.5) \cdot P_{rec}}{R \cdot T}$$

$$\rho_{mixrec}(T_{avg}) = 0.36422 \cdot \text{kg} \cdot \text{m}^{-3}$$

$$\text{Numavgrec7R6}(z) := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rerec6}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dcell6}} \right)^{0.8} \right]$$

CAPSTONE

$$\text{Numavgrec7R4}(z) = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rerec4}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dcell4}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{Numavgrec7R6}(\text{Lrec}) = 2.98024$$

$$\text{NumavgreccoR6}(z) = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rerec6}(\text{Tavg}) \cdot \text{Sc6T}(\text{Tavg}) \cdot \text{dcell6}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{NumavgR6}(\text{Lrec}) = 2.98441$$

$$\text{NumavgreccoR4}(z) = 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot z}{\text{Rerec4}(\text{Tavg}) \cdot \text{Sc6T}(\text{Tavg}) \cdot \text{dcell4}} \right)^{\frac{1}{3}} \right]^8$$

$$\text{NumavgreccoR4}(\text{Lrec}) = 2.97663$$

The average (integral) Nusselt numbers at 1-atm with the larger flow cross section show very little contribution of the thermal entry length, i.e. the flow velocities and heat and mass transfer coefficients have values close to those in long channels.

Now determine CH₄, C₇H₁₄, and CO conversions in 400 and 600 cpi honeycombs, assuming 80% C₇H₁₄ conversion downstream of the combustion monolith and upstream of the turbine

$$\text{ych4rec6}(T, z) := \text{ych4}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec6}(z)}{\text{Rerec6}(T) \cdot \text{ScT}(T) \cdot \text{dcell6}}\right)$$

$$\frac{\text{ych4rec6}(\text{Tavg}, \text{Lrec})}{\text{ych4}(\text{Tavg}, \text{Lhc})} = 2.733018 \cdot 10^{-13}$$

$$\text{ych4rec6}(\text{Tin}, \text{Lrec}) = 0 \quad \text{ych4}(\text{Tavg}, \text{Lhc}) = 1.81356 \cdot 10^{-5} \quad \text{Bypass} = 0 \quad \text{Lhc} = 3.5 \text{ in} \quad \text{Dia} = 9 \text{ in}$$

$$\text{yc7h14rec6}(T, z) := 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec7R6}(z)}{\text{Rerec6}(T) \cdot \text{Sc7T}(T) \cdot \text{dcell6}}\right)$$

$$\frac{\text{yc7h14rec6}(\text{Tin}, \text{Lrec})}{0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc})} = 0.00057$$

$$\text{yc7h14rec6}(\text{Tin}, \text{Lrec}) = 3.42819 \cdot 10^{-8} \quad 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) = 5.99172 \cdot 10^{-5}$$

$$\text{ych4rec4}(T, z) := \text{ych4}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec4}(z)}{\text{Rerec4}(T) \cdot \text{ScT}(T) \cdot \text{dcell4}}\right)$$

$$\frac{\text{ych4rec4}(\text{Tavg}, \text{Lrec})}{\text{ych4}(\text{Tavg}, \text{Lhc})} = 6.945016 \cdot 10^{-9}$$

$$\text{ych4rec4}(\text{Tin}, \text{Lrec}) = 8.84152 \cdot 10^{-13}$$

$$\text{yc7h14rec4}(T, z) := 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) \cdot \exp\left(\frac{-4 \cdot z \cdot \text{Numavgrec7R4}(z)}{\text{Rerec4}(T) \cdot \text{Sc7T}(T) \cdot \text{dcell4}}\right)$$

$$\frac{\text{yc7h14rec4}(\text{Tin}, \text{Lrec})}{0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc})} = 0.00773$$

$$\text{yc7h14rec4}(\text{Tin}, \text{Lrec}) = 4.63263 \cdot 10^{-7} \quad 0.2 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) = 5.99172 \cdot 10^{-5} \quad 0.4 \cdot \text{yc7h14}(\text{Tavg}, \text{Lhc}) = 8.3884 \cdot 10^{-4}$$

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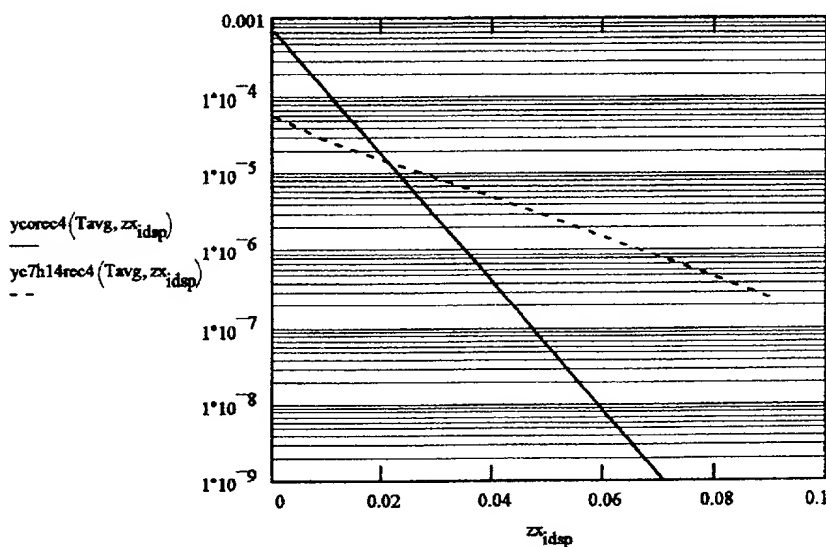
$$y_{corec4}(T,z) = 0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}) \cdot \exp\left(\frac{-4 \cdot z \cdot NumavgreccoR4(z)}{R_{rec4}(T) \cdot S_{ccoT}(T) \cdot d_{cell4}}\right)$$

$$y_{corec4}(T_{avg}, L_{rec}) = 3.06761 \cdot 10^{-11}$$

$$y_{corec6}(T,z) = 0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}) \cdot \exp\left(\frac{-4 \cdot z \cdot NumavgreccoR6(z)}{R_{rec6}(T) \cdot S_{ccoT}(T) \cdot d_{cell6}}\right)$$

$$y_{corec6}(T_{avg}, L_{rec}) = 2.9626 \cdot 10^{-15}$$

$$z_{x_{idsp}} := (idsp + 0.05) \cdot cm$$



$$Sc7T(T_{avg}) = 2.31842$$

$$S_{ccoT}(T_{avg}) = 0.73627$$

$$ScT(T_{avg}) = 0.67113$$

$$\frac{y_{corec4}(T_{avg}, L_{rec})}{(0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}))} = 3.65696 \cdot 10^{-8}$$

$$\frac{y_{corec6}(T_{avg}, L_{rec})}{(0.4 \cdot 7 \cdot y_{c7h14}(T_{avg}, L_{hc}))} = 3.53178 \cdot 10^{-12}$$

This analysis assumes 80% homogeneous conversion of fuel exiting a 3.5in. 600 cpi monolith without bypass flow and assuming 40% production of CO in the post combustion monolith region.

CO conversion in a 400 cpi recuperator monolith is >99.99%, while cyclohexane conversion is 99.2%.

The final CO and C7H14 levels are < 1 ppb and .5 ppm while post turbine concentrations are taken as 840 and 60 ppm respectively. CH4 conversion also should be very high and use of a 600 cpi or longer monolith would give higher HC conversions (x20 for 600 cpi).

Post turbine pre recuperation monolith pressure drops are modest: 0.56% for 400 cpi and 0.90% for 600 cpi monoliths.

An alternative method of calculating performance uses local Nusselt numbers for heat and mass transfer to determine the wall temperature and combustion rates at the wall. First we define the local Nu function then check conversion assuming fast kinetics and compare with the previous averaged (integrated) Nu formula.

Local Nu(x) taken from Kays & Crawford for hydro & thermal entrance laminar with circular channel:

$$\text{Numono}(z) := (1 + \exp(-1.09689 - 0.381402 \cdot \ln(z) - 8.287774 \cdot z^{0.5})) \cdot 3.6 \text{Numono}(0.1152163) = 3.82723$$

$$\text{zzchar6} := \frac{\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dcell6}}{2}$$

$$\text{zzchar6} = 8.90257 \cdot \text{cm}$$

$$\frac{\text{Lhc}}{\text{zzchar6}} = 0.99859$$

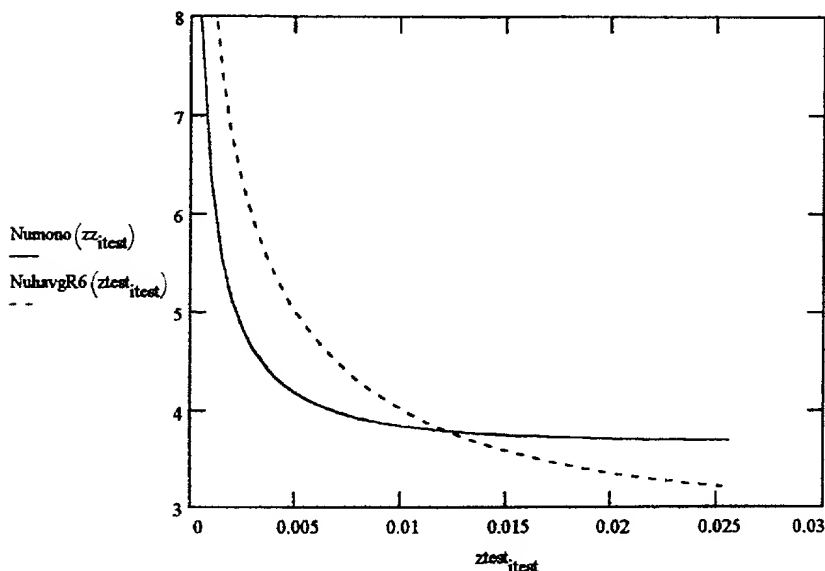
$$\text{Rehc6}(\text{Tavg}) = 252.34858$$

$$\text{itest} := 0..50$$

$$\text{dcell6} = 0.0967 \cdot \text{cm}$$

$$\text{ztest}_{\text{itest}} := \text{itest} \cdot 0.05 \cdot \text{cm} + 0.05 \cdot \text{cm}$$

$$\text{zz}_{\text{itest}} := \frac{\text{ztest}_{\text{itest}} + \text{dwall6}}{\text{zzchar6}}$$



$$\text{Rehc6}(\text{Tavg}) = 252.34858$$

$$\text{dcell6} = 0.0967 \cdot \text{cm}$$

$$\text{zz6ch4} := \frac{\text{Rehc6}(\text{Tavg}) \cdot \text{ScT}(\text{Tavg}) \cdot \text{dcell6}}{2}$$

$$\text{Pr}(.5, \text{Tavg}) = 0.72969$$

$$\text{Rehc6}(\text{Tavg}) \cdot \text{Pr}(.5, \text{Tavg}) \cdot \text{dcell6} = 17.80513 \cdot \text{cm}$$

$$\text{zz6c7h14} := \frac{\text{Rehc6}(\text{Tavg}) \cdot \text{Sc7T}(\text{Tavg}) \cdot \text{dcell6}}{2}$$

$$h(T, z) := \frac{\lambda_{\text{mix}} T(T) \cdot \text{Numono}\left(\frac{z}{\text{zzchar6}}\right)}{\text{dcell6}}$$

$$\text{kgpb}(T, z) := \frac{\text{Dch4T}(T) \cdot \text{Numono}\left(\frac{z}{\text{zz6ch4}}\right)}{\text{dcell6}}$$

$$\text{kgpb}(\text{Tin}, \text{Lhc}) = 15.5934 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$kgpb7(T, z) := \frac{Dc7h14T(T) \cdot Numono\left(\frac{z}{zz6c7h14}\right)}{dcell6}$$

$$kgpb7(Tin, Lhc) = 4.50626 \cdot \text{sec}^{-1} \cdot \text{cm}$$

Prater Temperature for CH4 at the inlet with fully developed flow

$$kgpb7(Tin, Lhc) \cdot \frac{P}{R \cdot Tin} \cdot \frac{ych40 \cdot \Delta H_{comb}(Tin)}{h(Tin, Lhc)} = 309.73474 \cdot K$$

Prater Temperature for C7H14 at the inlet with fully developed flow

$$kgpb7(Tin, Lhc) \cdot \frac{P}{R \cdot Tin} \cdot \frac{y0c7h14 \cdot \Delta H_{comb7}(Tin)}{h(Tin, 10 \cdot \text{cm})} = 90.38489 \cdot K$$

Determine maximum conversion of fuels with very fast catalytic combustion rates (zero fuel concentration at the wall)

$$iz := 0..100 \quad ych46_0 := ych40 \quad yc7h146_0 := y0c7h14 \quad T_{avg} = \frac{Tin + Tout}{2}$$

$$z6_{iz} := d_{wall6} + iz \cdot \frac{Lhc}{100} \cdot \frac{7}{7}$$

$$Lhc \cdot \frac{7}{7} = 8.89 \cdot \text{cm}$$

3.5 & 4-in. monolith length

$$ych46_{iz+1} := \left(1 - kgpb7(T_{avg}, z6_{iz}) \cdot \frac{Lhc}{100} \cdot \frac{7}{7} \cdot \frac{4}{dcell6} \cdot \frac{scell6}{U(T_{avg})}\right) \cdot ych46_{iz}$$

$$\frac{ych46_{101}}{ych40} = 1.2447 \cdot 10^{-4}$$

$$\frac{ych4\left(T_{avg}, Lhc \cdot \frac{7}{7}\right)}{ych40} = 0.00153$$

$$yc7h146_{iz+1} := \left(1 - kgpb7(T_{avg}, z6_{iz}) \cdot \frac{Lhc}{100} \cdot \frac{7}{7} \cdot \frac{4}{dcell6} \cdot \frac{scell6}{U(T_{avg})}\right) \cdot yc7h146_{iz}$$

$$\frac{yc7h146_{101}}{y0c7h14} = 0.06145$$

By-pass length yC7H14out/yin yCH4out/yin

0	3.5-in	0.06145	$1.2447 \cdot 10^{-4}$
0	4-in	0.04256	$3.288 \cdot 10^{-5}$
0.2	3.5-in	0.0502	$5.96324 \cdot 10^{-5}$
0.2	4-in	0.03374	$1.3974 \cdot 10^{-5}$
0.4	3.5-in	0.02054	$2.17587 \cdot 10^{-6}$
0.4	3.5-in	0.01207	$2.92928 \cdot 10^{-7}$

$$T_{avg} = 952.8725 \cdot K$$

$$Lhc = 3.5 \cdot \text{in}$$

$$Dia0 = 9 \cdot \text{in}$$

$$\text{Bypass} = 0$$

Nu function with circular channel hydrothermal entry length shows 93.9% to 98.8% conversion of C7H14

Packed bed

0495 FONG NICE

Pressure Drop Calculations for a Packed Bed

given: ϵ - void fraction;
 d_p - effective particle diameter
 U - mean superficial velocity
 ν - kinematic viscosity
 ρ - density

$$f_{bed}(x) := \frac{150}{x} + 1.75$$

$$x = \frac{150}{f_{bed}(x)}$$

1161 F

At $T = 900K$ and 10 atm pressure,

$$\rho_{mix}(0.0, 300K) = 3.47058 \cdot kg \cdot m^{-3}$$

$$\rho_{mix}(0.5, T_{avg}) = 1.09267 \cdot kg \cdot m^{-3} \quad \nu_{mix}(0.5, T_{avg}) = 0.00004 \cdot m^2 \cdot sec^{-1}$$

$$j := 0..3$$

$$d_{p_j} := \frac{0.125}{j+1} \cdot in$$

$$L_{bed} = 0.75 \cdot in$$

$$dp = \begin{bmatrix} 0.3175 \\ 0.15875 \\ 0.10583 \\ 0.07938 \end{bmatrix} \cdot cm$$

$$\epsilon := 0.5$$

$$\nu_0 := \nu_{mix}(0.5, T_{avg})$$

$$i := 1..10$$

$$U_{tx_i} := i \cdot m \cdot sec^{-1}$$

$$\rho_0 := \rho_{mix}(0.5, T_{avg})$$

$$Re_{bed_{i,j}} := U_{tx_i} \cdot \frac{d_{p_j}}{\nu_0 \cdot (1 - \epsilon)}$$

$$\Delta P_{i,j} := L_{bed} \cdot f_{bed}(Re_{bed_{i,j}}) \cdot \frac{1 - \epsilon}{\epsilon^3} \cdot \frac{\rho_0 \cdot (U_{tx_i})^2}{d_{p_j}}$$

$$U_{tx} = \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{matrix} \cdot m \cdot sec^{-1}$$

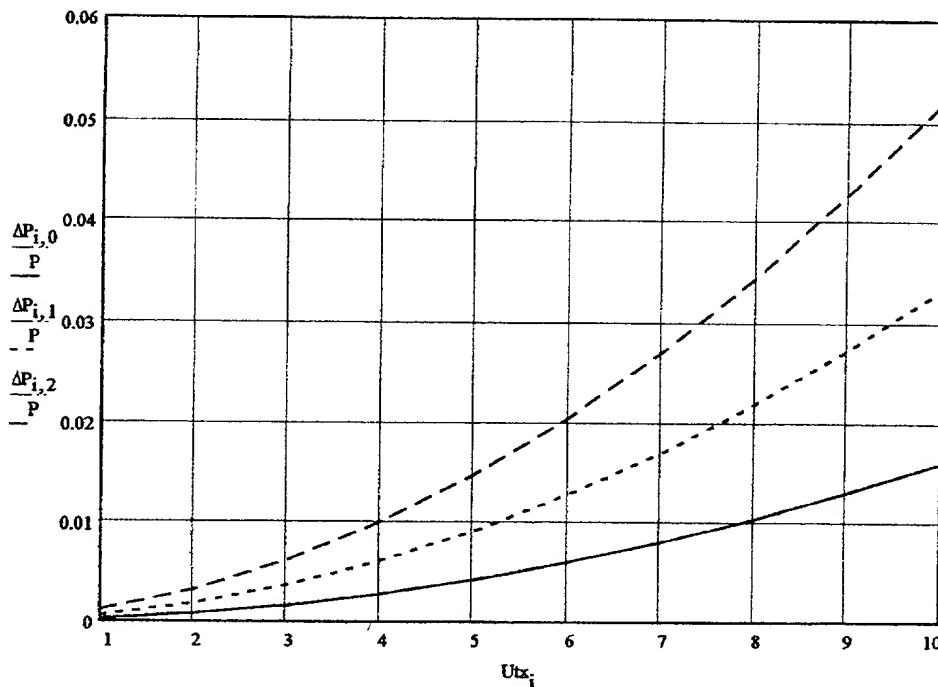
$$Re_{bed} =$$

0	0	0	0	0
1	175.19103	87.59551	58.39701	43.79776
2	350.38206	175.19103	116.79402	87.59551
3	525.57309	262.78654	175.19103	131.39327
4	700.76412	350.38206	233.58804	175.19103
5	875.95515	437.97757	291.98505	218.98875
6	1051.14617	525.57309	350.38206	262.78654
7	1226.3372	613.1686	408.77907	306.5843
8	1401.52823	700.76412	467.17608	350.38206
9	1576.71926	788.35963	525.57309	394.17982
10	1751.91029	875.95515	583.9701	437.97757

$$\Delta P =$$

0	0	0	0
0.00067	0.00179	0.00335	0.00536
0.00226	0.0054	0.00943	0.01434
0.00474	0.01081	0.01822	0.02695
0.00814	0.01804	0.02972	0.04318
0.01243	0.02708	0.04395	0.06304
0.01764	0.03794	0.0609	0.08651
0.02375	0.0506	0.08056	0.11362
0.03077	0.06508	0.10294	0.14435
0.03869	0.08137	0.12804	0.1787
0.04752	0.09947	0.15586	0.21668

$$\cdot atm$$



Particle diameter
 $dp_2 = 0.04167 \text{ in } \frac{1}{24}''$
 Smallest 1mm

$dp_1 = 0.0625 \text{ in } \frac{1}{16}''$

$dp_0 = 0.125 \text{ in } \frac{1}{8}''$

$L_{bed} = 0.75 \text{ in}$

$$\Delta P(\epsilon, T, z) := z \cdot f_{bed} \left[\frac{U_{bed}(T) \cdot dp_j}{v_0 \cdot (1 - \epsilon)} \right] \cdot \frac{1 - \epsilon \cdot \rho_0 \cdot (U_{bed}(T))^2}{\epsilon^3 \cdot dp_j} \quad \epsilon = 0.45$$

$$dp = \begin{bmatrix} 0.3175 \\ 0.15875 \\ 0.10583 \\ 0.07938 \end{bmatrix} \text{ cm}$$

$$\frac{\Delta P(.45, T_{avg}, L_{bed})}{P}$$

0.00173
0.00407
0.00703
0.0106

$$\frac{\Delta P(.5, T_{avg}, L_{bed})}{P}$$

0.00113
0.00263
0.00449
0.00673

$$U_{bed}(T_{avg}) = 2.5 \cdot \text{m} \cdot \text{sec}^{-1}$$

For larger particles use axial beds with greater length

$$k = 0$$

$$dp_0 = 0.125 \text{ in}$$

$\frac{1}{8}''$
 $\frac{1}{8}''$

which we have

$$U(T_{avg}) = 8.22528 \cdot \text{m} \cdot \text{sec}^{-1}$$

$$\Delta P_{axial}(\epsilon, T, z) := z \cdot f_{bed} \left[\frac{U(T) \cdot dp_k}{v_0 \cdot (1 - \epsilon)} \right] \cdot \frac{1 - \epsilon \cdot \rho_0 \cdot (U(T))^2}{\epsilon^3 \cdot dp_k}$$

$$\Delta P_{axial}(\epsilon, T_{avg}, 1 \text{ in}) = 0.0657 \text{ atm}$$

$$P = 3 \text{ atm}$$

$$\frac{\Delta P_{axial}(\epsilon, T_{avg}, 1 \text{ in})}{P} = 0.0219$$

1/8th inch pellets give about 2% pressure drop per inch

Determine Nu values for heat and mass transfer between particles and the gas phase in the bed

$$\text{Repart}(T) := \frac{U_{\text{bed}}(T) \cdot d_p}{v_{\text{mix}}(T) \cdot (1 - \varepsilon)}$$

$$d_p = \begin{bmatrix} 0.3175 \\ 0.15875 \\ 0.10583 \\ 0.07938 \end{bmatrix} \cdot \text{cm} \quad \varepsilon = 0.45$$

$$\text{Repart}(T_{\text{avg}}) = \begin{bmatrix} 398.16156 \\ 199.08078 \\ 132.72052 \\ 99.54039 \end{bmatrix} \quad \text{Pr}(.5, T_{\text{avg}}) = 0.72969 \quad \text{Sc}(.5, T_{\text{avg}}) = 0.67112$$

$$k := 0$$

$$\text{NuhpartR}(T) := 1.34 \cdot \left[\text{Pr}(.5, T)^{0.4} \cdot \left[0.4 \cdot (\text{Repart}(T)_k)^{0.5} + 0.2 \cdot (\text{Repart}(T)_k)^2 \right] \right]$$

$$\text{NuhpartR}(T_{\text{avg}}) = 22.21552$$

$$\text{havgpart}(T) = \frac{\lambda_{\text{mix}}(T) \cdot \text{NuhpartR}(T)}{d_{p_k}}$$

$$\text{havgpart}(T_{\text{avg}}) = 445.59219 \cdot \text{m}^{-2} \cdot \text{K}^{-1} \cdot \text{W}$$

Effective boundary layer thickness: $\frac{d_{p_k}}{\text{NuhpartR}(T_{\text{avg}})} = 142.9181 \cdot \mu\text{m}$

$$\frac{d_{\text{cell6}}}{\text{NuhavgR6}(\text{Lhc})} = 323.77508 \cdot \mu\text{m}$$

$$d_{p_k} = 0.3175 \cdot \text{cm}$$

$$d_{\text{cell6}} = 0.0967 \cdot \text{cm}$$

$$\text{NumpartR}(T) := 1.34 \cdot \text{Sc}(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repart}(T)_k)^2 + 0.2 \cdot (\text{Repart}(T)_k)^3 \right]$$

$$\text{NumpartR}(T_{\text{avg}}) = 21.48438$$

$$\text{kgpart}(T) := \frac{D_{\text{ch4}}(T) \cdot \text{NumpartR}(T)}{\varepsilon d_{p_k}}$$

$$\text{kgpart}(T_{\text{in}}) = 72.76151 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{Nupart7R}(T) := 1.34 \cdot \text{Sc7}(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repart}(T)_k)^{0.5} + 0.2 \cdot (\text{Repart}(T)_k)^2 \right]$$

$$\text{Nupart7R}(T_{\text{avg}}) = 35.27582$$

$$\text{kgfb7}(T) := \frac{D_{\text{c7h14}}(T) \cdot \text{Nupart7R}(T)}{\varepsilon d_{p_k}}$$

$$\text{kgfb7}(T_{\text{in}}) = 34.44665 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$ych46_{iz+1} := \left[1 - kgpart(Tavg) \cdot \frac{Lbed}{50} \cdot \frac{6 \cdot (1 - \varepsilon)^2}{dp_k} \cdot \frac{1}{Ubed(Tavg)} \right] \cdot ych46_{iz}$$

$$\frac{ych46_{51}}{ych46_0} = 0.02369771$$

$$ych4p(T, z) := ych40 \cdot \exp \left[-6 \cdot (1 - \varepsilon) \cdot \frac{NupartR(T)}{\varepsilon \cdot Reart(T)_k \cdot ScT(T)} \cdot \frac{z}{dp_k} \right]$$

$$\frac{ych4p(Tavg, Lbed)}{ych40} = 0.02908261$$

$$yc7h14(T, z) := y0c7h14 \cdot \exp \left[-6 \cdot (1 - \varepsilon) \cdot \frac{Nupart7R(T)}{\varepsilon \cdot Reart(T)_k \cdot Sc7T(T)} \cdot \frac{z}{dp_k} \right]$$

$$\frac{yc7h14(Tavg, Lbed)}{y0c7h14} = 0.18611$$

$$dp_k = 0.3175 \cdot \text{cm}$$

$$Ubed(Tavg) = 2.5 \cdot \text{m} \cdot \text{sec}^{-1}$$

$$\varepsilon = 0.45$$

$$Wbed = 17.78 \cdot \text{cm}$$

$$Lbed = 1.905 \cdot \text{cm}$$

dpart(cm)	yout/yinC7H14	yout/yinCH4	ΔP/P
0.3175	0.18611	0.02908261	0.00113
0.15875	0.0116	0.0000846	0.00263

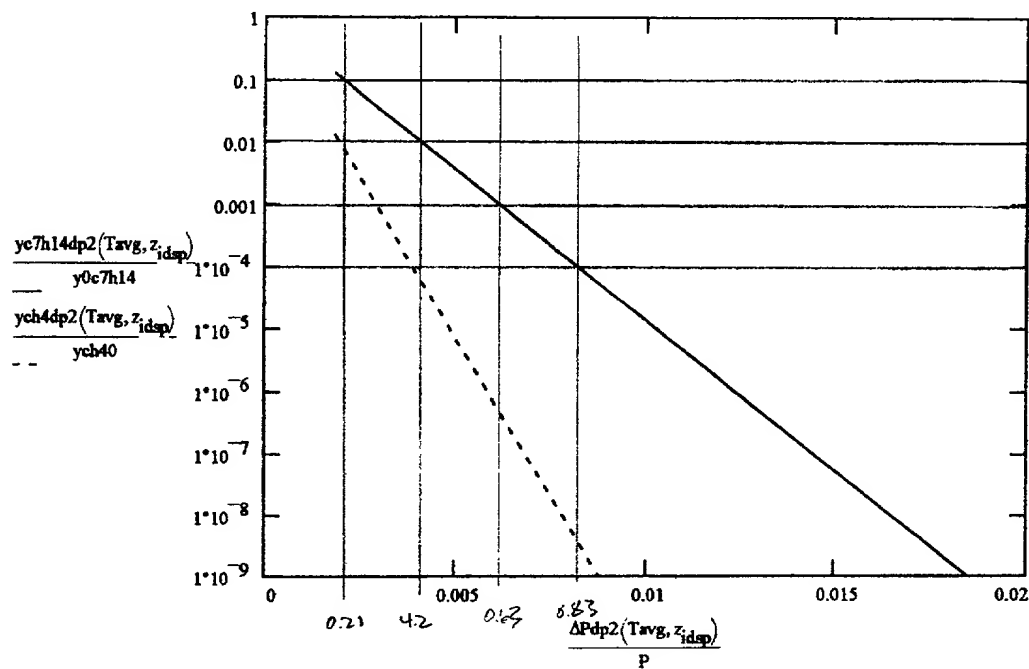
Determine hydrocarbon conversions in the packed beds vs pressure to estimate effective conversion at equivalent pressure drop

$$yc7h14dp2(T, z) := y0c7h14 \cdot \exp \left[-6 \cdot (1 - \varepsilon) \cdot \frac{1.34 \cdot Sc7T(T)^{0.4} \cdot \left[0.4 \cdot (Reart(T)_2)^2 + 0.2 \cdot (Reart(T)_2)^3 \right]}{\varepsilon \cdot Reart(T)_2 \cdot Sc7T(T)} \cdot \frac{z}{dp_2} \right]$$

$$ych4dp2(T, z) := ych40 \cdot \exp \left[-6 \cdot (1 - \varepsilon) \cdot \frac{1.34 \cdot ScT(T)^{0.4} \cdot \left[0.4 \cdot (Reart(T)_2)^2 + 0.2 \cdot (Reart(T)_2)^3 \right]}{\varepsilon \cdot Reart(T)_2 \cdot ScT(T)} \cdot \frac{z}{dp_2} \right]$$

$$\Delta Pdp2(Tavg, z) := z \cdot fbed(Reart(Tavg)_2) \cdot \frac{1 - \varepsilon}{\varepsilon^3} \cdot \frac{\rho_0 \cdot (Ubed(Tavg))^2}{dp_2}$$

$$Ubed(Tavg) = 2.5 \cdot \text{m} \cdot \text{sec}^{-1}$$



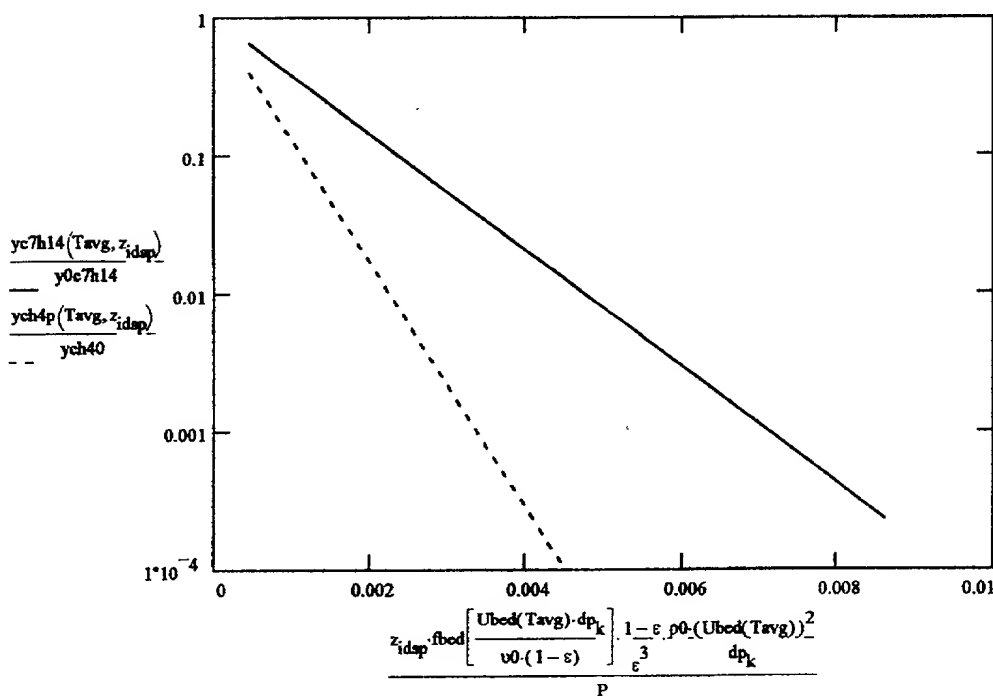
Small

$$dp_2 = 0.10583 \text{ cm}$$

$$dp_2 = 0.04167 \text{ in}$$

$$z_9 = 3.74016 \text{ in}$$

$$L_{bed} = 0.75 \text{ in}$$



Large

$$dp_0 = 0.3175 \text{ cm}$$

$$dp_0 = 0.125 \text{ in}$$

$$z_9 = 3.74016 \text{ in}$$

$$L_{bed} = 0.75 \text{ in}$$

$$U_{bed}(T_{avg}) = 2.5 \text{ m} \cdot \text{sec}^{-1}$$

For oblique flow through cone-shaped beds, large particles give a very low ΔP (even with thick beds) and high conversion

CAPSTONE PROJECT

$$z_{xx} := 2.71 \cdot \text{cm}$$

$$\frac{\Delta P_{dp2}(\text{Tavg}, z_{xx})}{P} = 0.01000$$

$$\frac{y_{c7h14dp2}(\text{Tavg}, z_{xx})}{y_{0c7h14}} = 1.32434 \cdot 10^{-5}$$

$$\frac{y_{ch4dp2}(\text{Tavg}, z_{xx})}{y_{ch40}} = 5.45793 \cdot 10^{-11}$$

For $\Delta P/P = 1\%$, C7H14 conversion = 99.9987% with fine particles, $dp = 1.06 \text{ mm}$

$$z_y := 2.0 \cdot \text{cm}$$

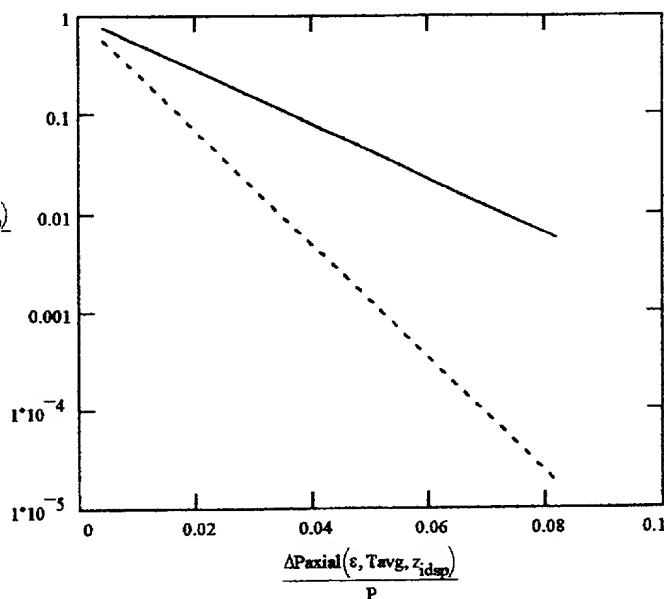
$$\text{Repaxial}(T) := \frac{U(T) \cdot dp_0}{u_{mix}T(T) \cdot (1 - \epsilon)}$$

$$\text{Numpaxial}(T) := 1.34 \cdot \text{Sc}T(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repaxial}(T))^1 + 0.2 \cdot (\text{Repaxial}(T))^2 \right]$$

$$\text{Nump7axial}(T) := 1.34 \cdot \text{Sc}7T(T)^{0.4} \cdot \left[0.4 \cdot (\text{Repaxial}(T))^1 + 0.2 \cdot (\text{Repaxial}(T))^2 \right]$$

$$y_{ch4paxial}(T, z) := y_{ch40} \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{\text{Numpaxial}(T)}{\epsilon \cdot \text{Repaxial}(T) \cdot \text{Sc}T(T)} \cdot \frac{z}{dp_0} \right]$$

$$y_{c7h14paxial}(T, z) := y_{0c7h14} \cdot \exp \left[-6 \cdot (1 - \epsilon) \cdot \frac{\text{Nump7axial}(T)}{\epsilon \cdot \text{Repaxial}(T) \cdot \text{Sc}7T(T)} \cdot \frac{z}{dp_0} \right]$$



Pressure drop increases approximately with the square of flow velocity while conversion decreases exponentially

$$U(\text{Tavg}) = 8.22528 \cdot \text{m} \cdot \text{sec}^{-1}$$

$$z_y := 2.32 \cdot \text{cm}$$

$$\frac{\Delta P_{axial}(\epsilon, \text{Tavg}, z_y)}{P} = 0.02000$$

$$\frac{y_{ch4paxial}(\text{Tavg}, z_y)}{y_{ch40}} = 0.06888284$$

$$\frac{y_{c7h14paxial}(\text{Tavg}, z_y)}{y_{0c7h14}} = 0.28038$$

For flow perpendicular to the fixed bed, even with large catalyst particles, the equivalent pressure drop for high C7H14 conversion is very high. Even with $\Delta P/P = 2\%$, the C7H14 conversion is only 72%. For high conversion with practical fixed beds, the superficial bed flow rate must lower than about 3 m/sec to give high conversion with low ΔP

CAPSTONE (ACT)

Define Catalyst Functions:

$$R = 82.07601 \cdot K^{-1} \cdot atm \cdot cm^3 \quad atm \cdot cm^3 / mol \cdot K$$

$$TOL := 0.0001$$

$$Rcm := 83143000 \cdot gm \cdot cm^2 \cdot sec^{-2} \cdot K^{-1}$$

$$\eta_{sph}(\phi) := \frac{3}{\phi} \cdot \left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi} \right)$$

$$\eta_{fpl}(\phi) := \frac{\tanh(\phi)}{\phi}$$

Physical Properties for Pd/Al₂O₃ Washcoated cCatalyst

$$Scat := 85 \cdot m^2 \cdot gm^{-1}$$

$$\rho_{catpart} := 2.5 \cdot gm \cdot cm^{-3}$$

$$V_{\mu pore} := 0.15 \cdot cm^3 \cdot gm^{-1}$$

$$Loat := 0.0020 \cdot cm$$

$$d_{pcat} := 0.0002 \cdot cm$$

Washcoat thickness - 20 microns

Size of γ -Al₂O₃ particle within washcoat - 2 microns

$$d_{\mu pore} := 6 \cdot \frac{V_{\mu pore}}{Scat}$$

$$\epsilon_{\mu pore} = 0.375$$

$$d_{\mu pore} = 1.05882 \cdot 10^{-6} \cdot cm$$

$$\tau_{\mu pore} := 3.0$$

$$DeffCH4(x, T) := \frac{\frac{\epsilon_{\mu pore}}{\tau_{\mu pore}}}{\frac{1}{Dch4(x, T)} + \frac{3}{d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot MW_0}}}}$$

$$d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot Tin}{\pi \cdot MW_0}} = 0.10953 \cdot sec^{-1} \cdot cm^2$$

$$Dch4(.5, Tin) = 0.41195 \cdot sec^{-1} \cdot cm^2$$

$$DeffCH4(.5, Tin) = 0.00419 \cdot sec^{-1} \cdot cm^2$$

$$DeffC7H14(x, T) := \frac{\frac{\epsilon_{\mu pore}}{\tau_{\mu pore}}}{\frac{1}{Dc7h14(x, T)} + \frac{3}{d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot T}{\pi \cdot MW_6}}}}$$

$$d_{\mu pore} \cdot \sqrt{\frac{8 \cdot R \cdot Tin}{\pi \cdot MW_6}} = 0.04428 \cdot sec^{-1} \cdot cm^2$$

$$Dc7h14(.5, Tin) = 0.11846 \cdot sec^{-1} \cdot cm^2$$

$$DeffC7H14(0.5, Tin) = 0.00164 \cdot sec^{-1} \cdot cm^2$$

T02230-09000000

$$D_{\text{macCH4}}(x, T) := \frac{0.4}{2.5} \cdot D_{\text{ch4}}(x, T)$$

$$D_{\text{macCH4}}(.5, 800 \cdot K) = 0.06442 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$D_{\text{macC7H14}}(x, T) := \frac{0.4}{2.5} \cdot D_{\text{c7h14}}(x, T)$$

$$D_{\text{macC7H14}}(.5, 800 \cdot K) = 0.01851 \cdot \text{sec}^{-1} \cdot \text{cm}^2$$

$$k_0T := 0.01 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1} \text{ Test value for } k_0T$$

Macropore porosity - 0.4 and tortuosity - 2.5

Microscopic Thiele Modulus for CH4

$$\phi_{\mu}(k_0T, x, T) := \sqrt{\left[\rho_{\text{catpart}} \cdot \left(\frac{R \cdot T}{P_{\text{ref}}} \right) \cdot \frac{k_0T}{D_{\text{effCH4}}(x, T)} \right] \cdot \frac{d_{\text{pcat}}}{6}}$$

$$\phi_{\mu}(k_0T, .5, T_{\text{in}}) = 0.021$$

Macroscopic Thiele Modulus for CH4

$$\Phi_{\text{mac}}(k_0T, x, T) := \sqrt{\left[\rho_{\text{catpart}} \cdot \left(\frac{R \cdot T}{P_{\text{ref}}} \right) \cdot k_0T \right] \cdot \frac{\eta_{\text{sph}}(\phi_{\mu}(k_0T, x, T))}{D_{\text{macCH4}}(x, T)} \cdot L_{\text{cat}}}$$

$$\Phi_{\text{mac}}(k_0T, y_{\text{ch40}}, T_{\text{in}}) = 0.31774$$

Microscopic Thiele Modulus for C7H14

$$\phi_{\mu 7}(k_0T, x, T) := \sqrt{\left[\rho_{\text{catpart}} \cdot \left(\frac{R \cdot T}{P_{\text{ref}}} \right) \cdot \frac{k_0T}{D_{\text{effC7H14}}(x, T)} \right] \cdot \frac{d_{\text{pcat}}}{6}}$$

$$\phi_{\mu 7}(k_0T, .5, T_{\text{in}}) = 0.03357$$

Macroscopic Thiele Modulus for C7H14

$$\Phi_{\text{mac7}}(k_0T, x, T) := \sqrt{\left[\rho_{\text{catpart}} \cdot \left(\frac{R \cdot T}{P_{\text{ref}}} \right) \cdot k_0T \right] \cdot \frac{\eta_{\text{sph}}(\phi_{\mu 7}(k_0T, x, T))}{D_{\text{macC7H14}}(x, T)} \cdot L_{\text{cat}}}$$

$$\Phi_{\text{mac7}}(k_0T, y_{\text{ch40}}, T_{\text{in}}) = 0.59265$$

$$\text{RatekCH4}(k_0T, x, T) := -\eta_{\text{sph}}(\phi_{\mu}(k_0T, x, T)) \cdot \eta_{\text{fp}}(\Phi_{\text{mac}}(k_0T, x, T)) \cdot \left[\rho_{\text{catpart}} \cdot \left(\frac{R \cdot T}{P_{\text{ref}}} \right) \cdot k_0T \right]$$

$$\text{RatekCH4}(k_0T, 0, T_{\text{in}}) = -1610.07113 \cdot \text{sec}^{-1}$$

$$\text{RatekC7H14}(k_0T, x, T) := -\eta_{\text{sph}}(\phi_{\mu 7}(k_0T, x, T)) \cdot \eta_{\text{fp}}(\Phi_{\text{mac7}}(k_0T, x, T)) \cdot \left[\rho_{\text{catpart}} \cdot \left(\frac{R \cdot T}{P_{\text{ref}}} \right) \cdot k_0T \right]$$

$$\text{RatekC7H14}(k_0T, 0, T_{\text{in}}) = -1492.98186 \cdot \text{sec}^{-1}$$

Defines transport restricted rate constant function given catalyst effective first order rate constant - k_0T , methane or cyclohexane conversion - x , and surface temperature - T

$$Ts := Tin \quad k0T = 0.01 \cdot \text{sec}^{-1} \cdot \text{gm}^{-1} \quad T_{avg} = 952.8725 \cdot \text{K}$$

$$kgpb(Tin, 0.1 \cdot \text{cm}) = 26.77306 \cdot \text{sec}^{-1} \cdot \text{cm} \quad \text{RatekCH4}(k0T, 0, Ts) = -1610.07113 \cdot \text{sec}^{-1} \quad Lcat = 0.002 \cdot \text{cm}$$

$$Tin + \frac{kgpb(T_{avg}, 0.1 \cdot \text{cm})}{\left[\frac{kgpb(T_{avg}, 0.1 \cdot \text{cm})}{- \text{RatekCH4}(k0T, 0, Ts) \cdot Lcat} + 1 \right]} \cdot \frac{ych40 \cdot -\Delta H_{comb}(T_{avg})}{h(T_{avg}, 0.1 \cdot \text{cm})} \cdot \frac{P}{R \cdot Ts} = 840.46756 \cdot \text{K} \quad T_{out} = 1094.817 \cdot \text{K}$$

$$xs := ych40 \quad xs = 0.01183 \quad T_{in} = 810.928 \cdot \text{K}$$

$$Rk := 6.33 \cdot \text{m}^{-2} \cdot \text{sec}^{-1} \quad \text{Ratech4} := 0.036 \cdot \text{m}^{-2} \cdot \text{sec}^{-1} \quad k0T = 10 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

Set up subroutine/function to solve for the surface temperature given a rate constant

$$TOL := 0.0001 \quad ych40 = 0.01183 \quad x := 0.01$$

$$Ts := 1673 \cdot \text{K} \quad Ts7 := 1473 \cdot \text{K}$$

Given

$$Ts = Tin + \frac{y(ych40, x)_0 \cdot \frac{P}{R \cdot Ts} - \Delta H_{comb}(Ts)}{\frac{1}{- \text{RatekCH4}(k0T, x, Ts) \cdot Lcat} + \frac{1}{kgpb\left(Tin, \frac{Lhc}{100}\right)} h\left(Tin, \frac{Lhc}{100}\right)}$$

$$Tshi(k0T) := \text{Find}(Ts) \quad Tshi(100 \cdot k0T) = 1010.10631 \cdot \text{K}$$

Given

$$Ts7 = Tin + \frac{y7(y0c7h14, x)_6 \cdot \frac{P}{R \cdot Ts} - \Delta H_{comb7}(Ts)}{\frac{1}{- \text{RatekC7H14}(k0T, x, Ts) \cdot Lcat} + \frac{1}{kgpb7\left(Tin, \frac{Lhc}{100}\right)} h\left(Tin, \frac{Lhc}{100}\right)}$$

$$Tshi7(k0T) := \text{Find}(Ts7) \quad Tshi7(100 \cdot k0T) = 873.32275 \cdot \text{K}$$

$$Rk := - \text{RatekCH4}(k0T, xs, Ts) \cdot Lcat$$

$$Rk7 := - \text{RatekC7H14}(k0T, xs, Ts) \cdot Lcat$$

$$Rk = 6.72632 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$Rk7 = 6.41773 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$k0T = 10 \cdot \text{kg}^{-1} \cdot \text{sec}^{-1}$$

$$\text{Ratech4} := \frac{xs \cdot \frac{P}{R \cdot Ts}}{\frac{1}{Rk} + \frac{1}{kgpb(Tin, Lhc)}}$$

$$kgpb(Tin, Lhc) = 15.5934 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$\text{Ratech4} = 0.01215 \cdot \text{m}^{-2} \cdot \text{sec}^{-1}$$

$$kgpb7(Tin, Lhc) = 4.50626 \cdot \text{sec}^{-1} \cdot \text{cm}$$

$$Ts := Tin + Ratech4 \cdot \frac{-\Delta H_{comb}(Ts)}{h(Tin, Lhc)} \cdot ych40$$

$$Ratech4 = 0.01215 \cdot m^{-2} \cdot sec^{-1}$$

$$xs := \frac{Ratech4}{Rk}$$

$$Rk = 6.72632 \cdot sec^{-1} \cdot cm$$

$$Ts = 811.4626 \cdot K$$

$$xs = 0.18057 \cdot m^{-3}$$

$$Tin = 810.928 \cdot K$$

$$k0T = 10 \cdot kg^{-1} \cdot sec^{-1}$$

$$Tshi(100 \cdot k0T) = 1010.10631 \cdot K$$

$$Tshi(0.01 \cdot kg^{-1} \cdot sec^{-1}) = 810.96346 \cdot K$$

$$Tshi7(100 \cdot k0T) = 873.32275 \cdot K$$

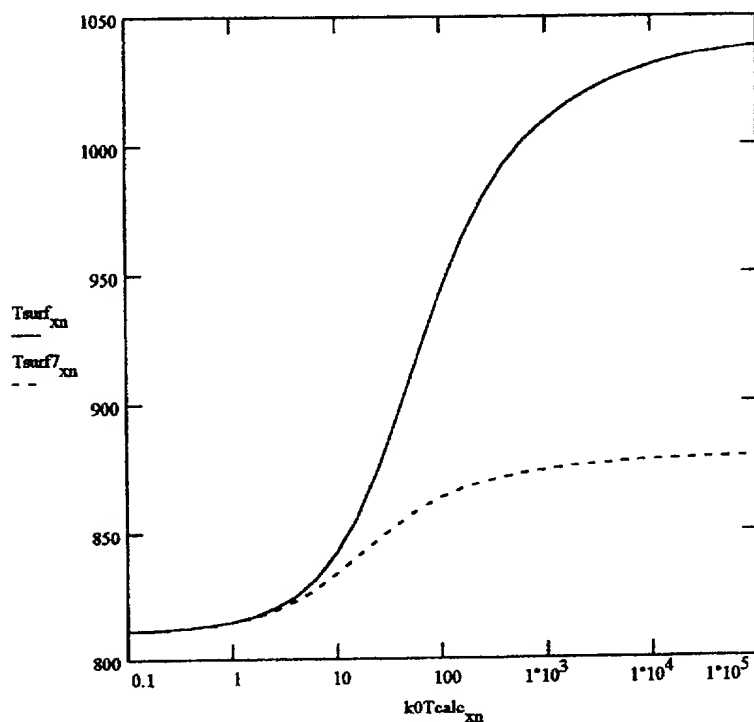
$$Tshi7(0.01 \cdot kg^{-1} \cdot sec^{-1}) = 810.96393 \cdot K$$

$$xn := 0, 1 \dots 30$$

$$k0Tcalc_{xn} := 10^{-1 + \frac{xn}{5}} \cdot kg^{-1} \cdot sec^{-1}$$

$$Tsurf_{xn} = Tshi(k0Tcalc_{xn})$$

$$Tsurf7_{xn} = Tshi7(k0Tcalc_{xn})$$



This plot shows the surface temperature within a honeycomb channel as a function of the specific catalytic rate constant for methane and methylcyclohexane combustion at a location within 1-mm of the leading edge

Takes into account the internal pore diffusion (micro- and macropores) and boundary layer heat and mass transport. Upper surface temperature limit approaches the adiabatic temperature for methane and a much lower (Prater) temperature for C7H14

k0 unit - sec⁻¹ per kg washcoat
T unit - K

We can also determine the actual effective first order rate constants for methane, propane, and other fuels and estimate the temperatures required for catalytic light-off and extinction, with roughly estimated Nu numbers.

Other factors, such as the upstream surface temperature and gas phase radial temperature profile and thermal conduction of the catalyst wall, can also effect the light-off and the critical extinction points. These calculations are beyond the scope of the current analysis.

PdO Catalyst Rate Constants

$$\text{Erpd0} := 12800 \cdot \text{K} \quad \text{Erpd1} := 4900 \cdot \text{K} \quad \text{Erpd3} := 15000 \cdot \text{K}$$

Region0 - low T PdO to 625K
ignores inhibition by H₂O and CO₂

Region1 - Intermediate T
625K to 909K

Region2 - Flat 909K
to 1048K decomposition

Region3 -
Pd metal

$$\text{Apd0} := 2.4 \cdot 10^3 \cdot 200 \cdot \text{gm}^{-1} \cdot \text{sec}^{-1}$$

$$\text{Apd1} := \text{Apd0} \cdot \exp\left(-\frac{\text{Erpd0}}{625 \cdot \text{K}} + \frac{\text{Erpd1}}{625 \cdot \text{K}}\right)$$

$$\text{Apd2} := \text{Apd1} \cdot \exp\left(\frac{-\text{Erpd1}}{909.1 \cdot \text{K}}\right)$$

$$\text{Apd3} := \text{Apd2} \cdot \exp\left(\frac{\text{Erpd3}}{1048.1 \cdot \text{K}}\right)$$

Interpolation formula for the four PdO+Pd rate constants

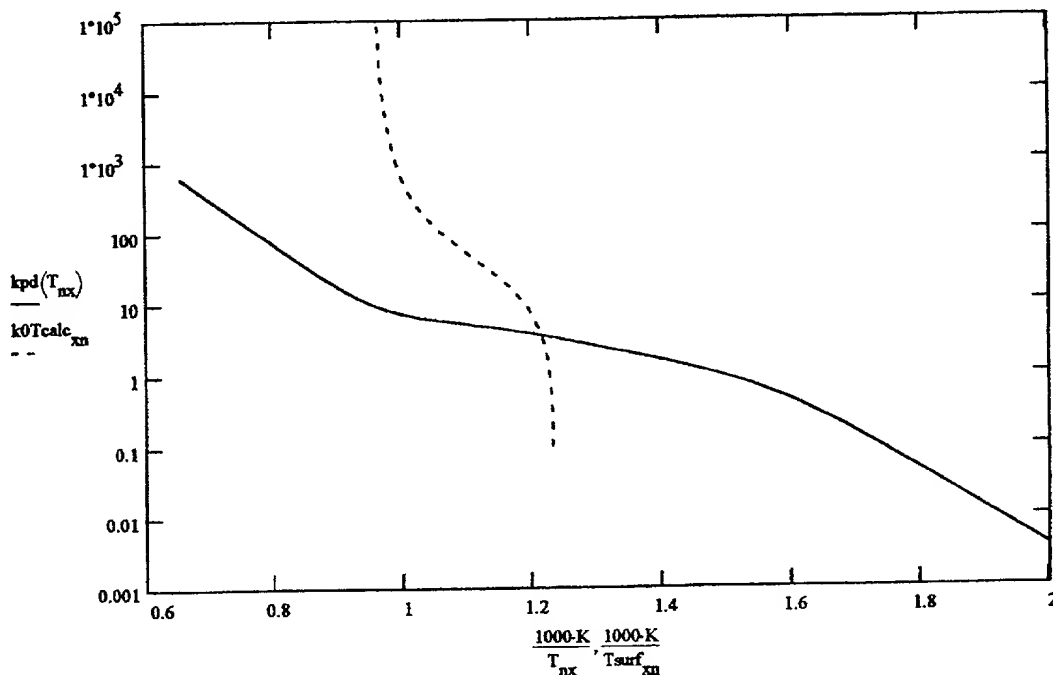
$$k_{pd}(T) := \left[\text{Apd3}^2 \cdot \exp\left(-\frac{2 \cdot \text{Erpd3}}{T}\right) + \frac{1}{\left(\text{Apd2}^{-2} + \text{Apd1}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd1}}{T}\right) + \text{Apd0}^{-2} \cdot \exp\left(\frac{2 \cdot \text{Erpd0}}{T}\right) \right)} \right]^{0.5}$$

$$n_x := 0, 1, \dots, 41 \quad T_{nx} := 500 \cdot \text{K} + n_x \cdot 25 \cdot \text{K}$$

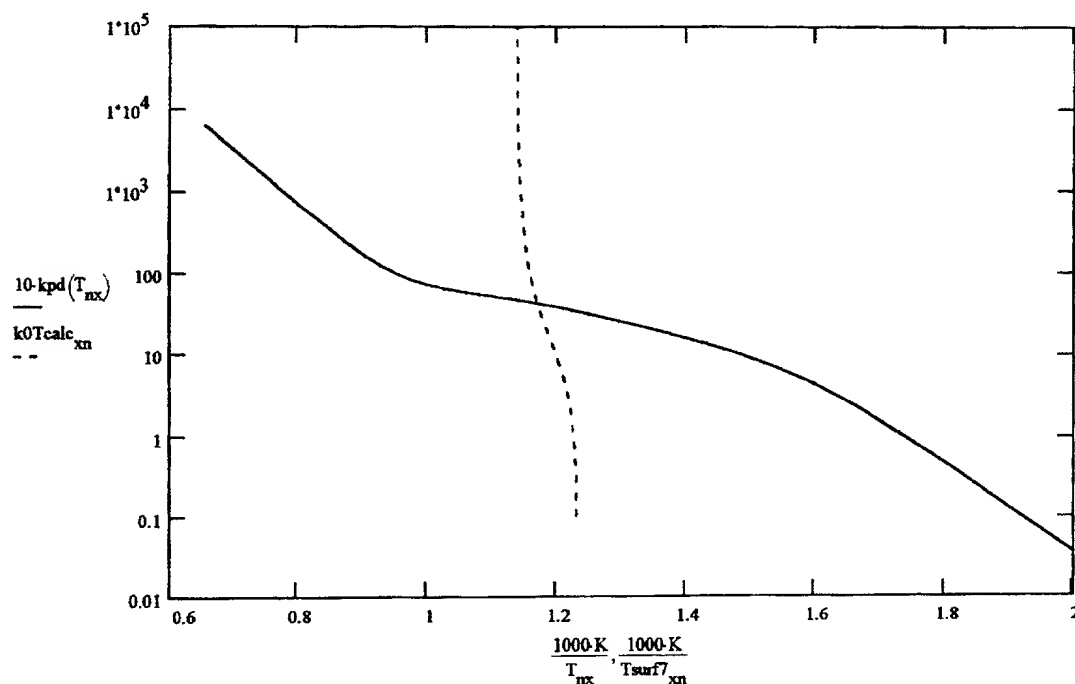
CATALYTIC RATE CONSTANT NEEDED FOR HEAT BALANCE IN A MONOLITH WITH FULLY DEVELOPED FLOW

Compared with extrapolated but measured rate constants (mol/atmCH₄/s/gcat)

$$L_{cat} = 0.00002 \cdot \text{m}$$



Compared with extrapolated and estimated
rate constants for C7H14 (10x mol/atmCH4/s/gcat)



Define functions to calculate surface temperature profiles given gas temperature and composition

$$TOL := 0.1 \quad Ts = 811.4626 \cdot K$$

$$x = 0.01$$

$$Tsx := 1500 \cdot K \quad Tsx7 := 1400 \cdot K$$

$$\frac{1}{-RatekCH4(kpd(Tsx), x, Tsx) \cdot Lcat} + \frac{1}{kgpb(Tin, Lhc)} = 7.01896 \cdot m^{-1} \cdot sec$$

Given

$$Tsx = Tin + \frac{y(ych40, x)_0 \cdot \frac{P}{R \cdot Tsx} - \frac{\Delta H_{comb}(Tsx)}{h(Tin, z)}}{\frac{1}{-RatekCH4(kpd(Tsx), x, Tsx) \cdot Lcat} + \frac{1}{kgpb(Tin, z)}}$$

$$Tsrf(Tin, x, z) := Find(Tsx)$$

$$Tsch4x := Tsrf(Tin, x, 0.1 \cdot cm)$$

$$Z \text{ inlet} = 0.1 \text{ cm}$$

$$Tsch4x = 823.23891 \cdot K$$

$$Tin = 810.928 \cdot K$$

$$x = 0.01$$

$$Lcat = 0.002 \cdot cm$$

$$y(ych40, x)_0 = 0.01171$$

$$kpd(Tsch4x) = 3.51311 \cdot kg^{-1} \cdot sec^{-1}$$

$$kgpb(Tin, 0.1 \cdot cm) = 26.77306 \cdot sec^{-1} \cdot cm$$

$$-RatekCH4(kpd(Tsch4x), x, Tsch4x) \cdot Lcat = 1.17316 \cdot sec^{-1} \cdot cm$$

Given

$$T_{sx7} = T_{in} + \frac{y_7(y_{0c7h14}, x)_6 \cdot \frac{P}{R \cdot T_{sx7}} - \Delta H_{comb7}(T_{sx7})}{\frac{1}{-Rate_{kC7H14}(10 \cdot kpd(T_{sx7}), x, T_{sx7}) \cdot L_{cat}} + \frac{1}{kg_{pb7}(T_{in}, z)} h(T_{in}, z)}$$

$$T_{srf7}(T_{in}, x, z) := Find(T_{sx7})$$

$$T_{sc7h14x} := T_{srf7}(T_{in}, x, 0.1 \cdot cm)$$

$$Z_{inlet} = 0.1 \cdot cm$$

$$T_{sc7h14x} = 871.51735 \cdot K$$

$$T_{in} = 810.928 \cdot K$$

$$x = 0.01$$

$$L_{cat} = 0.002 \cdot cm$$

$$y(y_{ch40}, x)_0 = 0.01171$$

$$10 \cdot kpd(T_{sc7h14x}) = 44.23122 \cdot kg^{-1} \cdot sec^{-1}$$

$$-Rate_{kC7H14}(10 \cdot kpd(T_{sc7h14x}), x, T_{sc7h14x}) \cdot L_{cat} = 9.21644 \cdot sec^{-1} \cdot cm$$

$$kg_{pb7}(T_{in}, 0.1 \cdot cm) = 12.3599 \cdot sec^{-1} \cdot cm$$

Assuming the rate constant for C7H14 combustion is ten times the rate constant for CH4 combustion, the surface temperature near the inlet (1-mm in) is 871.5 K (1100F) and near the transport limit for C7H14 and 823.2K (1050F) and surface rate controlled for CH4. If this calculation is repeated for a series of steps downstream with corrections to the gas phase concentrations and temperatures, new surface temperatures and rates can be calculated through the length of the monolith.

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